

Data Path : U:\HPCHEM1\BNA F\DATA\BF082117\
 Data File : BF097902.D
 Acq On : 21 Aug 2017 13:13
 Operator : SJ/JU
 Sample : I4849-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CAPTAINSCOVE-WC-002

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.157	175	182	196	rBV	165151	412340	7.88%	0.505%
2	4.957	483	488	498	rVB	318934	508811	9.72%	0.623%
3	5.363	551	557	560	rBV	3613806	4092010	78.16%	5.008%
4	6.392	719	732	735	rBV	3441002	4451958	85.04%	5.449%
5	6.522	748	754	757	rBV	3751455	4030744	76.99%	4.933%
6	6.745	789	792	796	rBV	1166902	958914	18.32%	1.174%
7	6.904	813	819	822	rBV	3196508	3092772	59.07%	3.785%
8	7.316	883	889	892	rBV	2493225	2711507	51.79%	3.319%
9	7.416	898	906	910	rBV	97001	150029	2.87%	0.184%
10	7.933	990	994	996	rBV	118317	122101	2.33%	0.149%
11	7.951	996	997	1003	rVV	81970	66775	1.28%	0.082%
12	8.028	1006	1010	1016	rBV	1430168	1276050	24.37%	1.562%
13	8.416	1072	1076	1081	rBV	166924	186474	3.56%	0.228%
14	8.828	1143	1146	1150	rVB2	69411	62362	1.19%	0.076%
15	9.110	1188	1194	1197	rBV	4012676	3952934	75.50%	4.838%
16	9.410	1241	1245	1248	rBV	126968	106970	2.04%	0.131%
17	9.498	1256	1260	1265	rVB	808129	734340	14.03%	0.899%
18	9.780	1301	1308	1311	rBV2	1440547	1268620	24.23%	1.553%
19	9.816	1311	1314	1317	rVB3	41848	54570	1.04%	0.067%
20	10.569	1437	1442	1445	rVB	2225571	2132687	40.74%	2.610%
21	10.692	1460	1463	1467	rBV	101455	121600	2.32%	0.149%
22	10.780	1474	1478	1481	rBV4	46347	54848	1.05%	0.067%
23	10.922	1499	1502	1510	rVB2	75101	102700	1.96%	0.126%
24	11.098	1530	1532	1535	rBV	88301	74175	1.42%	0.091%
25	11.139	1535	1539	1541	rBV	61391	52563	1.00%	0.064%
26	11.263	1556	1560	1562	rBV	1246982	1073944	20.51%	1.314%
27	11.298	1565	1566	1569	rVV	113364	106542	2.04%	0.130%
28	11.327	1569	1571	1577	rVB2	81925	80833	1.54%	0.099%
29	11.486	1594	1598	1604	rBV2	101015	105755	2.02%	0.129%
30	11.798	1647	1651	1654	rBV2	91037	96588	1.84%	0.118%
31	11.968	1678	1680	1690	rVB5	47447	73389	1.40%	0.090%
32	12.468	1761	1765	1768	rVB	206466	206259	3.94%	0.252%
33	12.604	1785	1788	1794	rVB	195525	171685	3.28%	0.210%
34	12.692	1798	1803	1807	rBV	144140	176492	3.37%	0.216%

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35	12.845	1825	1829	1833	rBV	2355323	2436954	46.55%	2.983%
36	13.057	1862	1865	1868	rBV3	95792	117178	2.24%	0.143%
37	13.086	1868	1870	1874	rVB3	113804	105368	2.01%	0.129%
38	13.410	1922	1925	1926	rBV3	60145	53571	1.02%	0.066%
39	13.427	1926	1928	1931	rVB	84968	70583	1.35%	0.086%
40	13.545	1945	1948	1951	rVB	96969	89472	1.71%	0.110%
41	13.745	1978	1982	1988	rBV2	860399	1211864	23.15%	1.483%
42	13.892	2001	2007	2010	rBV	989077	1043336	19.93%	1.277%
43	14.068	2032	2037	2040	rBV2	263163	355183	6.78%	0.435%
44	14.192	2055	2058	2061	rBV	409627	336331	6.42%	0.412%
45	14.380	2085	2090	2096	rBV	2740910	2775083	53.01%	3.396%
46	14.433	2097	2099	2103	rVB3	71284	77074	1.47%	0.094%
47	14.498	2107	2110	2114	rBV	184122	172014	3.29%	0.211%
48	14.674	2135	2140	2146	rBV2	424372	649519	12.41%	0.795%
49	14.745	2149	2152	2156	rVB2	128250	135106	2.58%	0.165%
50	14.815	2160	2164	2170	rVV	1650044	1676469	32.02%	2.052%
51	14.904	2176	2179	2182	rBV	72270	103382	1.97%	0.127%
52	15.009	2191	2197	2199	rBV	3349850	5235374	100.00%	6.408%
53	15.074	2205	2208	2218	rVB	306755	436723	8.34%	0.535%
54	15.157	2219	2222	2226	rBV	306959	357379	6.83%	0.437%
55	15.315	2244	2249	2252	rBV	630839	785518	15.00%	0.961%
56	15.357	2253	2256	2259	rVV	180409	241351	4.61%	0.295%
57	15.392	2259	2262	2266	rVV2	209579	274680	5.25%	0.336%
58	15.451	2269	2272	2279	rVB2	120319	182022	3.48%	0.223%
59	15.551	2284	2289	2300	rBV	1550305	2165209	41.36%	2.650%
60	15.780	2322	2328	2331	rBV	1158151	1873800	35.79%	2.293%
61	15.827	2331	2336	2342	rVV	2076655	3485655	66.58%	4.266%
62	15.892	2342	2347	2360	rVV	629368	1284042	24.53%	1.572%
63	16.004	2361	2366	2377	rVB2	342213	798875	15.26%	0.978%
64	16.151	2387	2391	2398	rVB4	124533	246391	4.71%	0.302%
65	16.315	2415	2419	2424	rBV2	123604	206318	3.94%	0.253%
66	16.533	2449	2456	2469	rBV	1268046	2505561	47.86%	3.067%
67	16.715	2483	2487	2497	rVB6	213975	455411	8.70%	0.557%
68	16.827	2498	2506	2511	rVV4	383550	1042196	19.91%	1.276%
69	16.898	2512	2518	2527	rVV	791838	1992373	38.06%	2.438%
70	16.986	2528	2533	2547	rVB	334061	934036	17.84%	1.143%
71	17.262	2572	2580	2590	rBV2	917134	2338252	44.66%	2.862%

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72	17.462	2610	2614	2626	rVB4	139079	342373	6.54%	0.419%
73	17.592	2628	2636	2647	rBV3	278376	1046268	19.98%	1.281%
74	17.692	2648	2653	2665	rVB6	181536	577399	11.03%	0.707%
75	17.792	2666	2670	2677	rVB5	103739	245694	4.69%	0.301%
76	17.874	2678	2684	2690	rBV3	232784	556484	10.63%	0.681%
77	18.015	2703	2708	2711	rBV5	97978	195261	3.73%	0.239%
78	18.150	2727	2731	2736	rBV6	89902	186834	3.57%	0.229%
79	18.227	2737	2744	2756	rVB3	359969	1107332	21.15%	1.355%
80	18.497	2785	2790	2798	rVB7	63522	158285	3.02%	0.194%
81	19.062	2874	2886	2900	rVB3	885034	2981455	56.95%	3.649%
82	19.227	2902	2914	2928	rVB2	980441	3188603	60.90%	3.903%

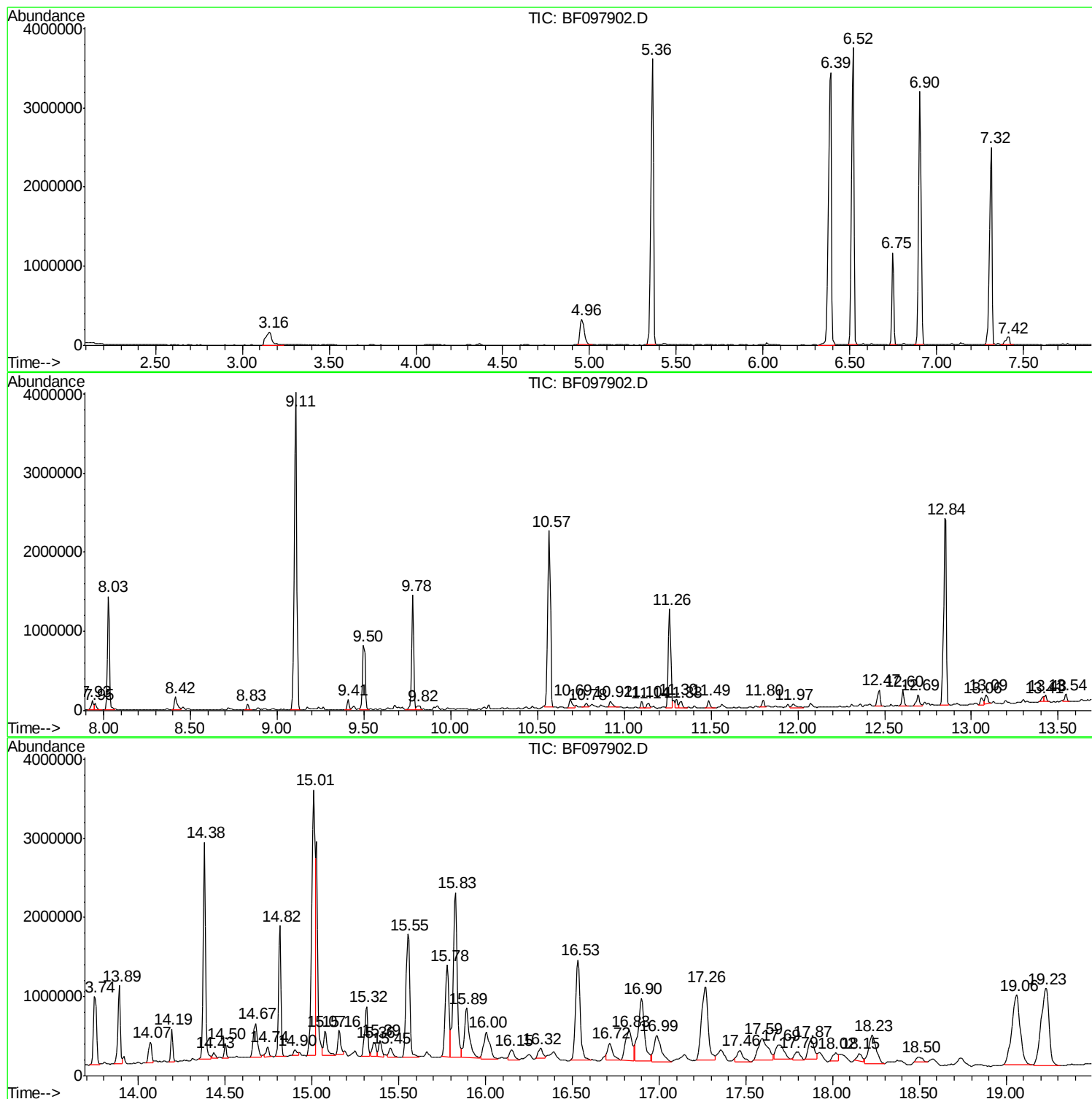
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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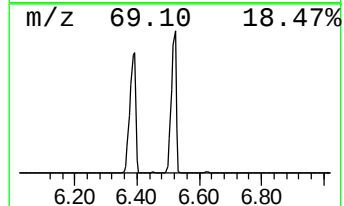
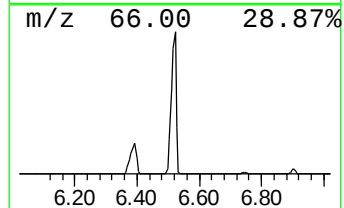
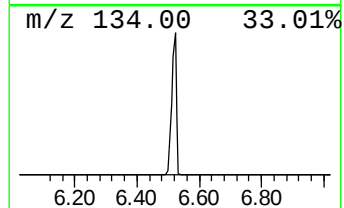
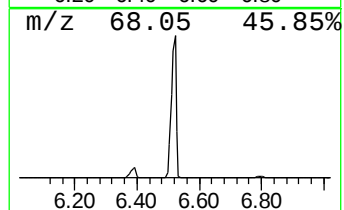
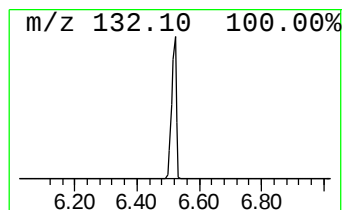
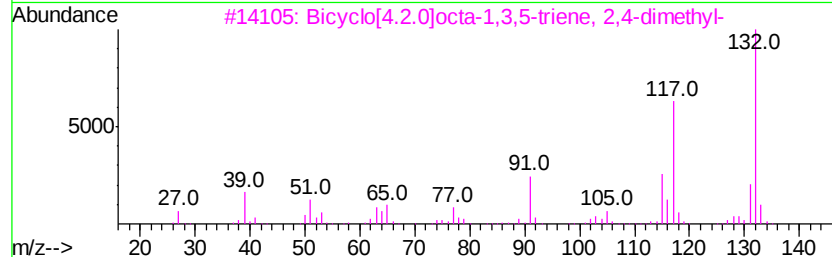
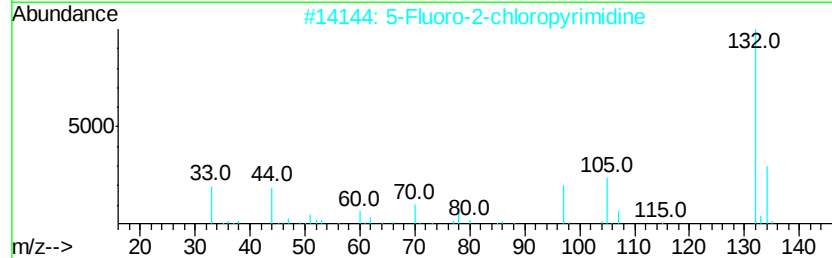
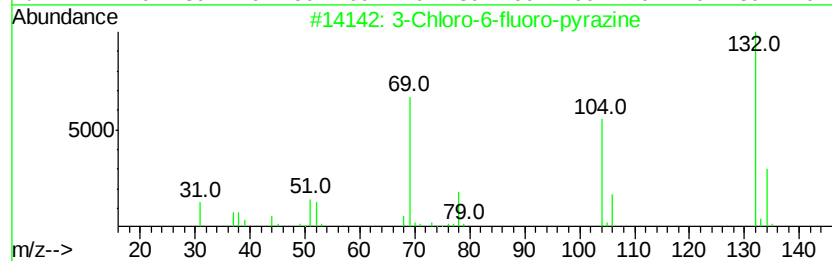
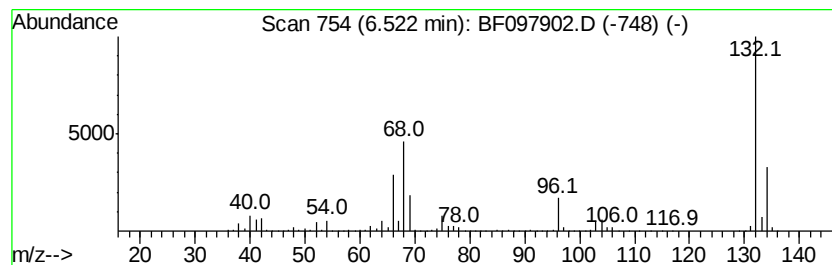
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.52 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	84.07 ng	4030740	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Xenon	132	Xe	007440-63-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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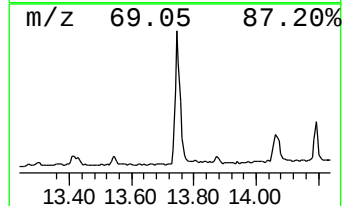
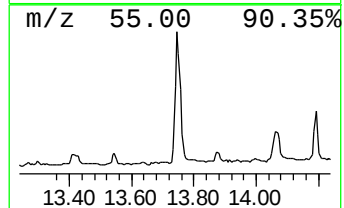
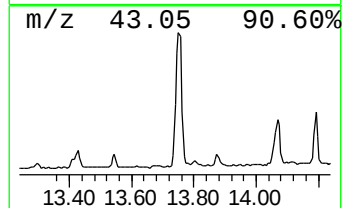
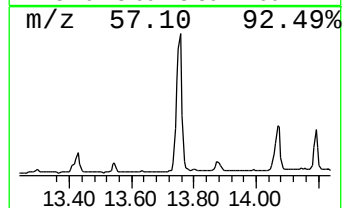
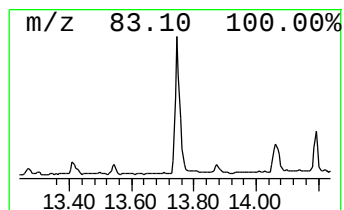
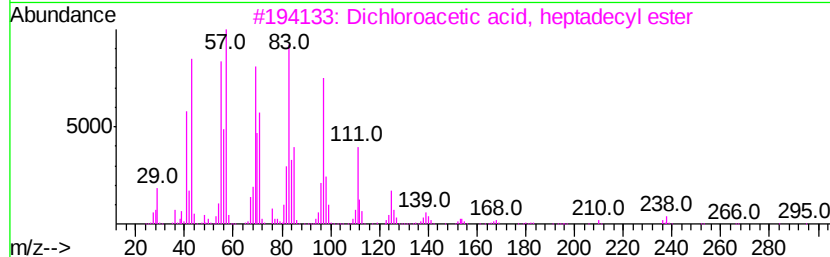
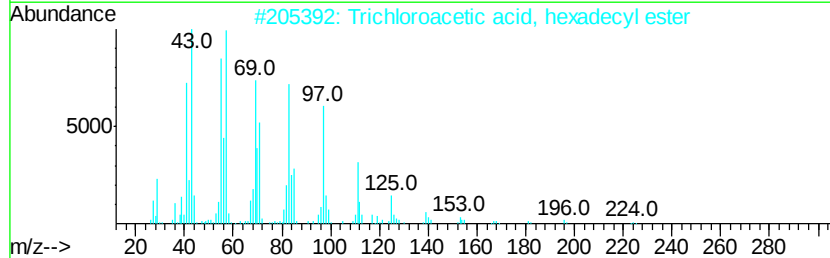
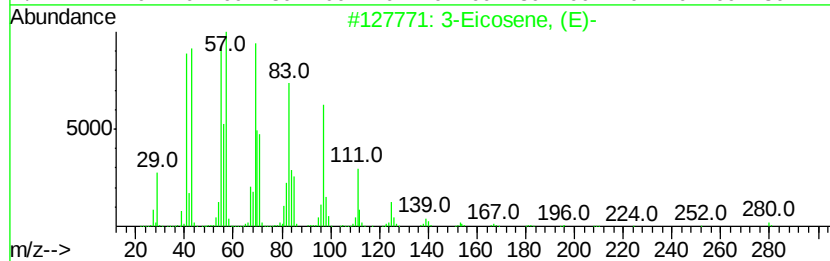
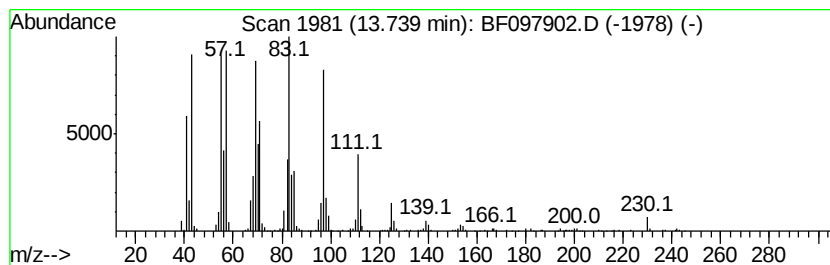
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 3-Eicosene, (E)- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	23.23 ng	1211860	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Eicosene, (E)-	280	C20H40	074685-33-9	99
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
4		1-Heneicosanol	312	C21H44O	015594-90-8	90
5		2-Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	90



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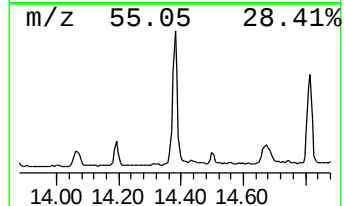
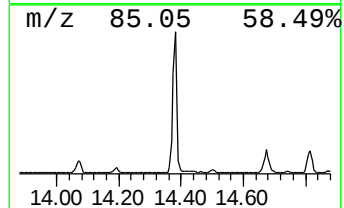
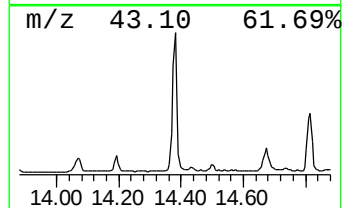
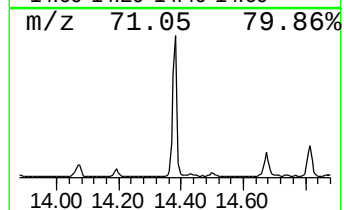
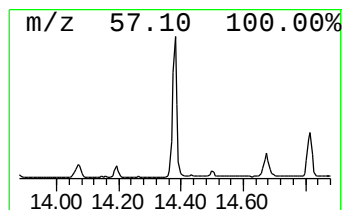
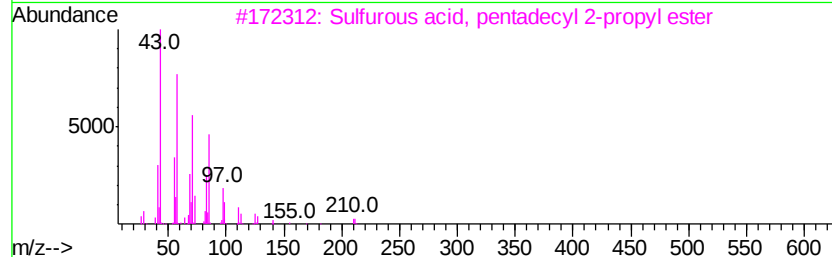
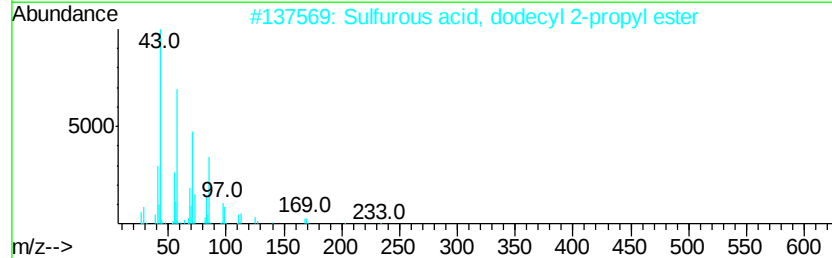
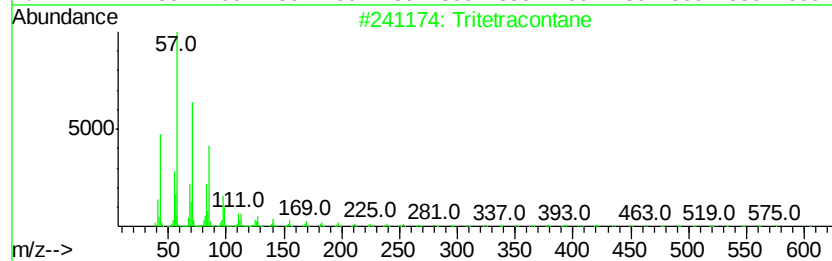
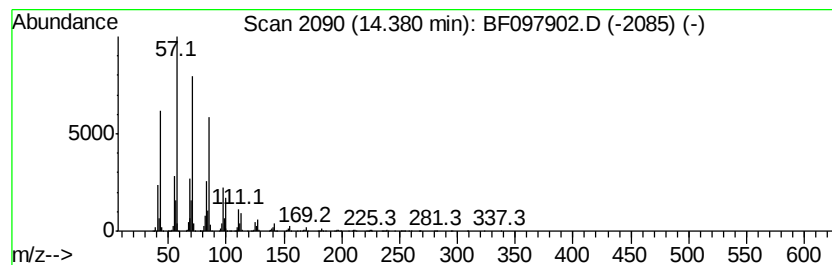
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Tritetracontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.38	53.20 ng	2775080	Chrysene-d12	13.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tritetracontane	605	C43H88	007098-21-7	91
2		Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	90
3		Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	90
4		Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	86
5		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	86



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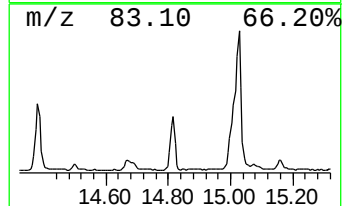
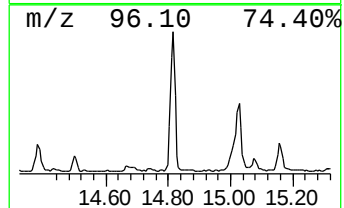
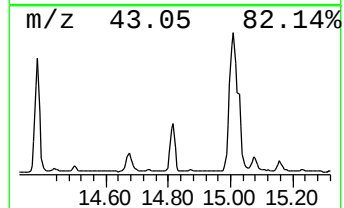
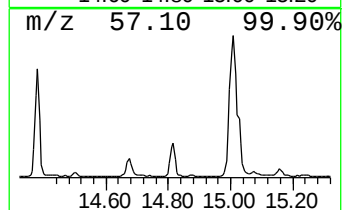
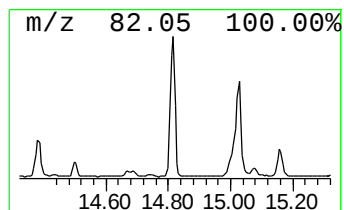
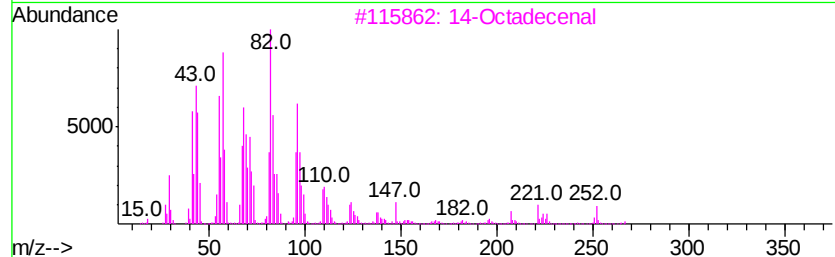
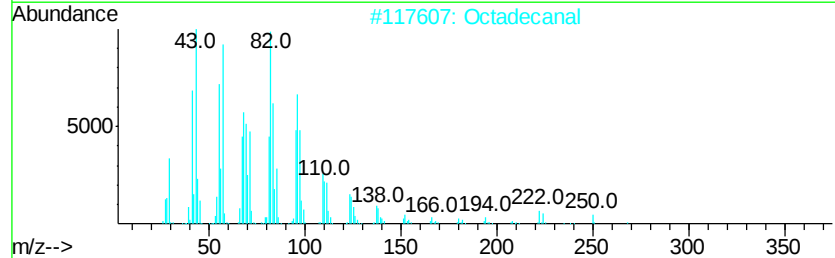
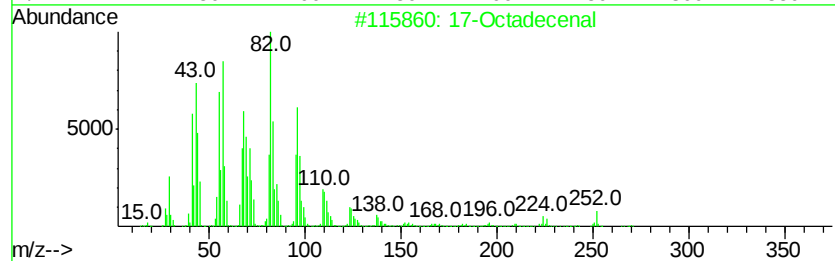
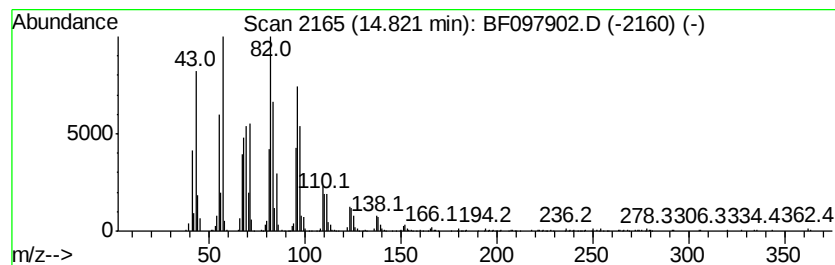
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 17-Octadecenal Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	42.68 ng	1676470	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	17-Octadecenal	266	C18H34O	056554-86-0	91
2		Octadecanal	268	C18H36O	000638-66-4	91
3		14-Octadecenal	266	C18H34O	056554-89-3	89
4		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
5		Pentadecanal-	226	C15H30O	002765-11-9	87



Data Path : U:\HPCHEM1\BNA F\DATA\BF082117\
Data File : BF097902.D
Acq On : 21 Aug 2017 13:13
Operator : SJ/JU
Sample : I4849-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

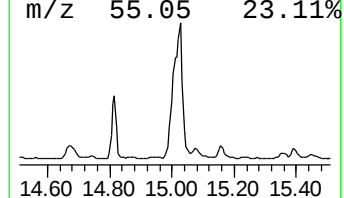
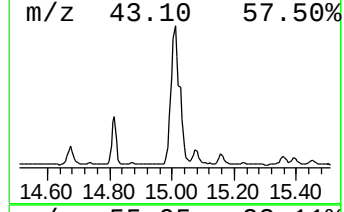
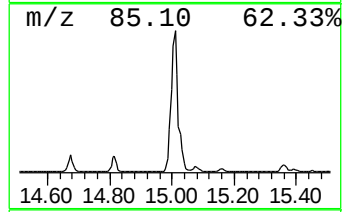
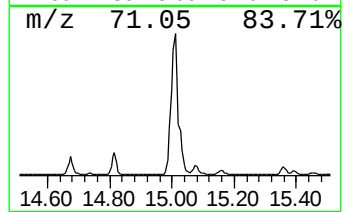
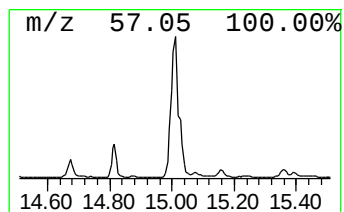
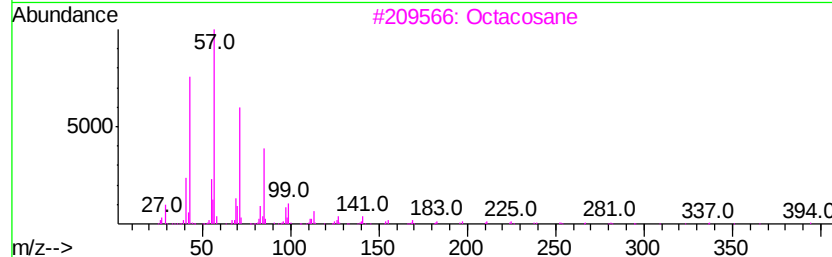
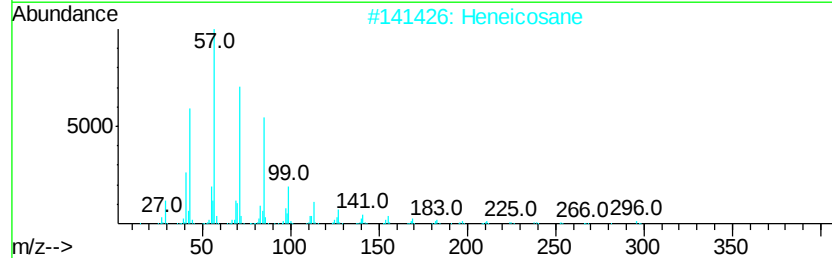
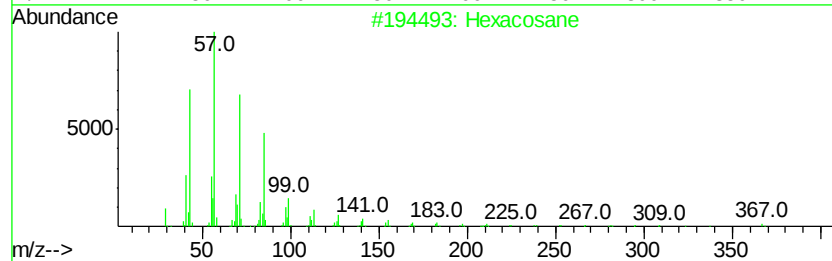
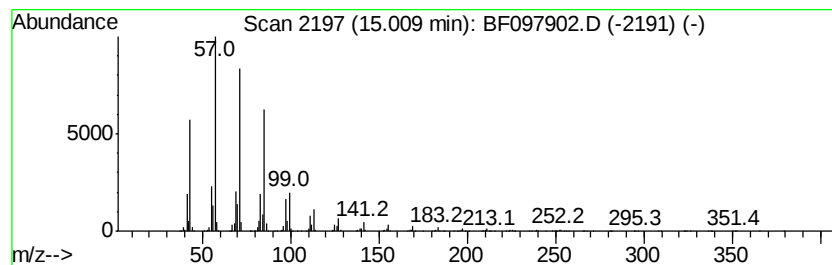
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexacosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.01	133.30 ng	5235370	Perylene-d12	15.32
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexacosane	366 C26H54	000630-01-3	87
2	Heneicosane	296 C21H44	000629-94-7	87
3	Octacosane	394 C28H58	000630-02-4	80
4	Tetratetracontane	619 C44H90	007098-22-8	74
5	Eicosane, 10-methyl-	296 C21H44	054833-23-7	72



Data Path : U:\HPCHEM1\BNA F\DATA\BF082117\
Data File : BF097902.D
Acq On : 21 Aug 2017 13:13
Operator : SJ/JU
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CAPTAINSCOVE-WC-002

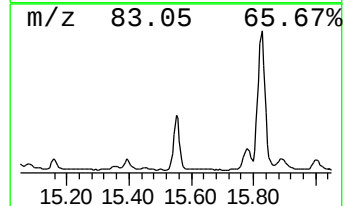
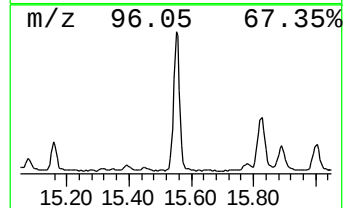
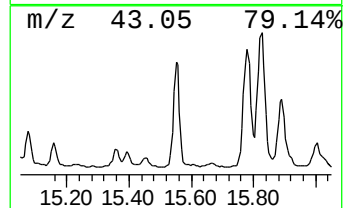
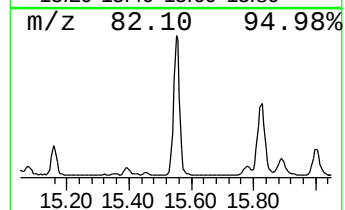
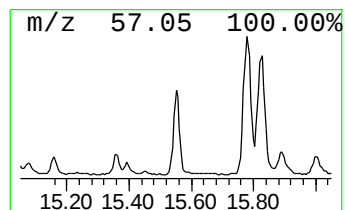
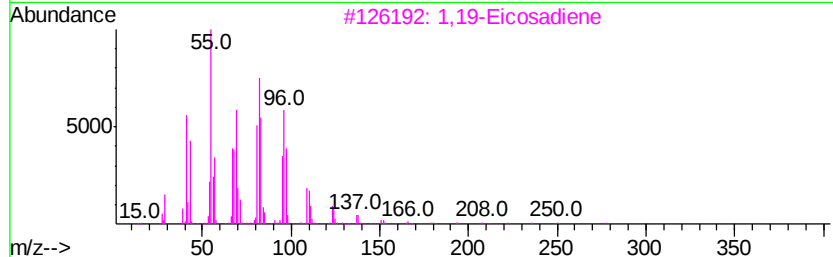
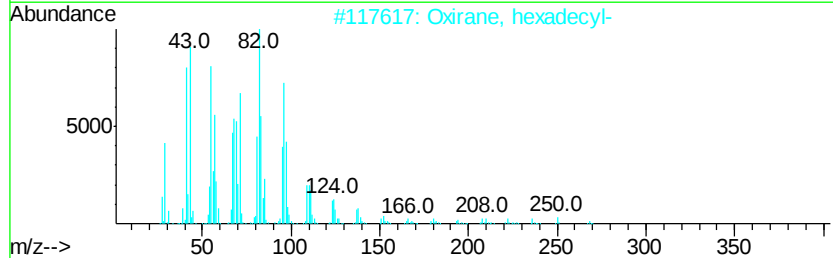
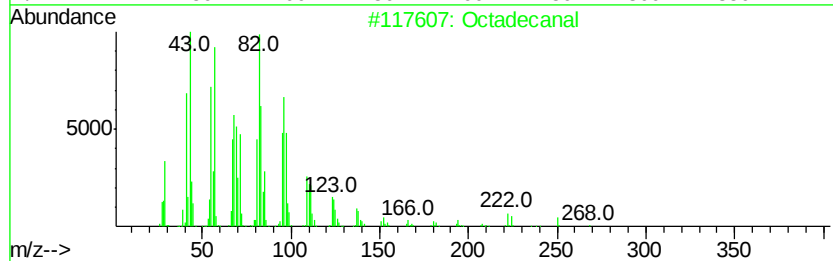
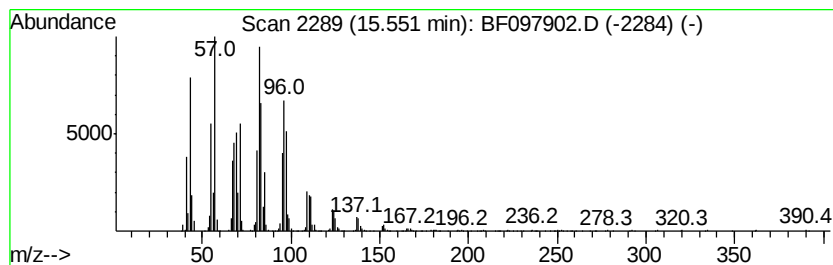
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.55	55.13 ng	2165210	Perylene-d12	15.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal		268	C18H36O	000638-66-4	91
2	Oxirane, hexadecyl-		268	C18H36O	007390-81-0	90
3	1,19-Eicosadiene		278	C20H38	014811-95-1	83
4	Hexadecanal		240	C16H32O	000629-80-1	80
5	1,16-Hexadecanediol		258	C16H34O2	007735-42-4	74



Data Path : U:\HPCHEM1\BNA F\DATA\BF082117\
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Acq On : 21 Aug 2017 13:13
Operator : SJ/JU
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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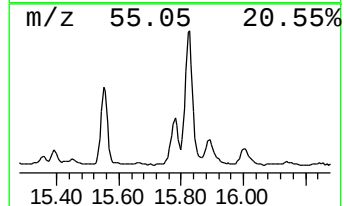
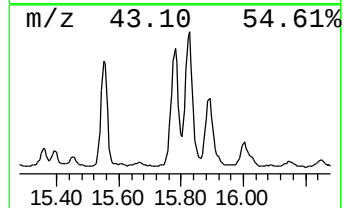
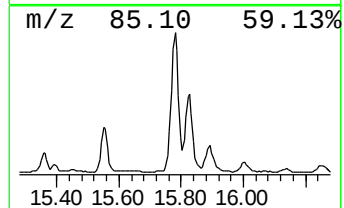
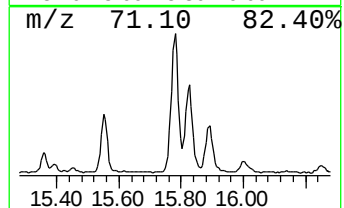
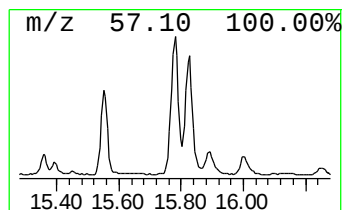
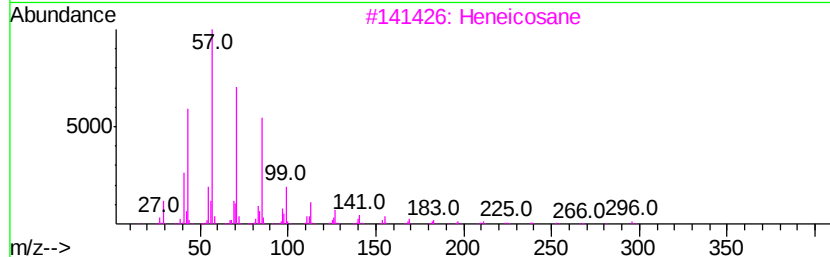
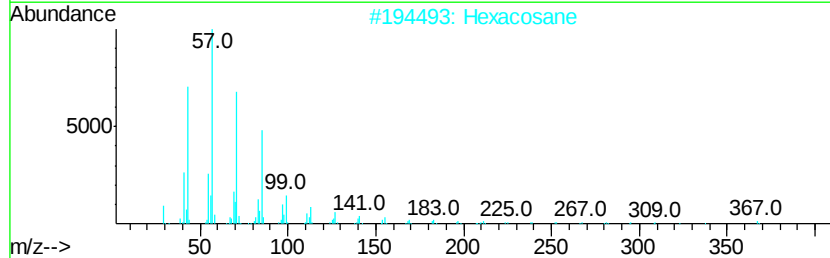
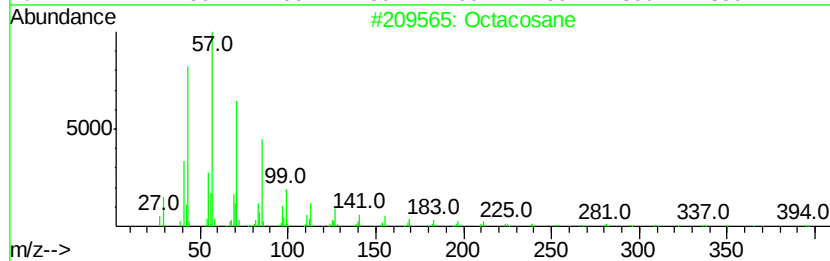
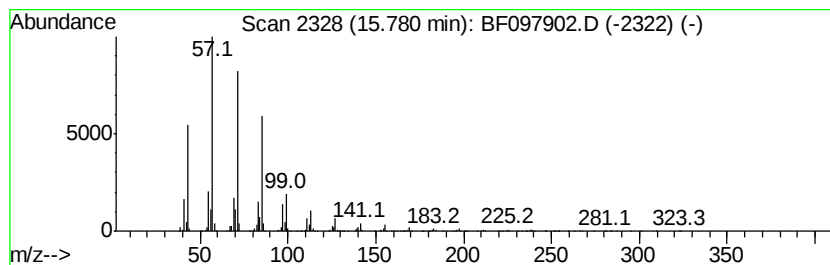
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Octacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.78	47.71 ng	1873800	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heneicosane	296	C21H44	000629-94-7	90
4		10-Methylnonadecane	282	C20H42	056862-62-5	90
5		Eicosane, 10-methyl-	296	C21H44	054833-23-7	86



Data Path : U:\HPCHEM1\BNA_F\DATA\BF082117\
Data File : BF097902.D
Acq On : 21 Aug 2017 13:13
Operator : SJ/JU
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Misc :
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Instrument :
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ClientSampleId :
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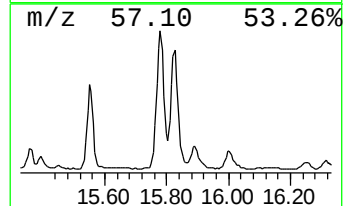
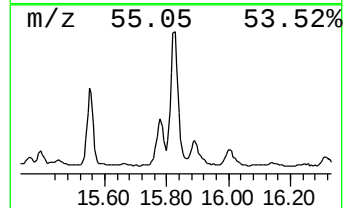
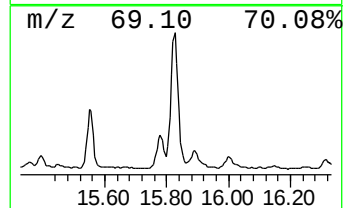
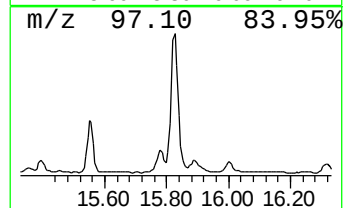
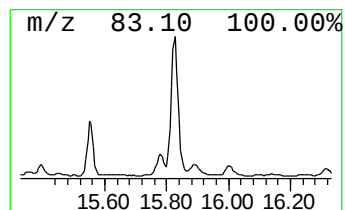
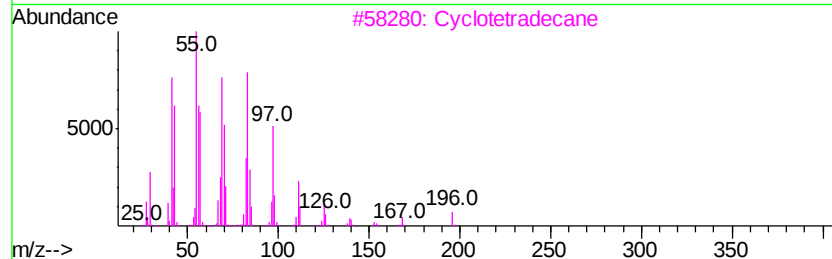
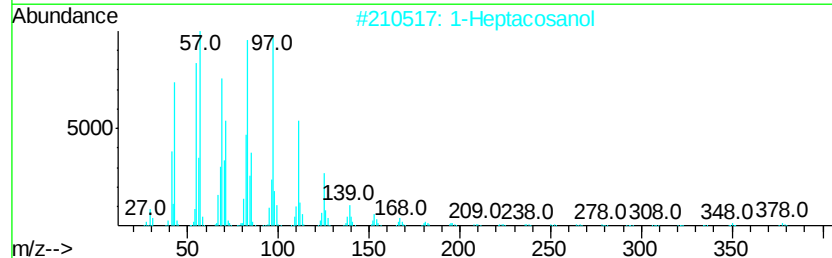
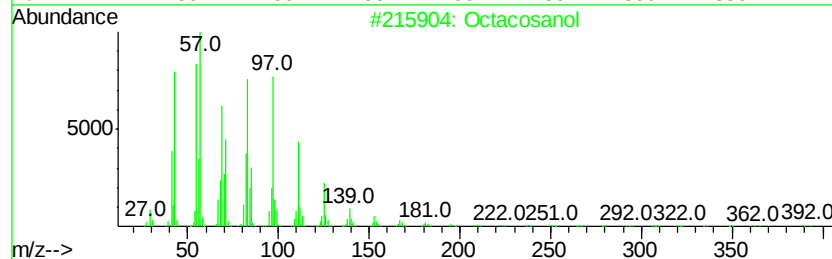
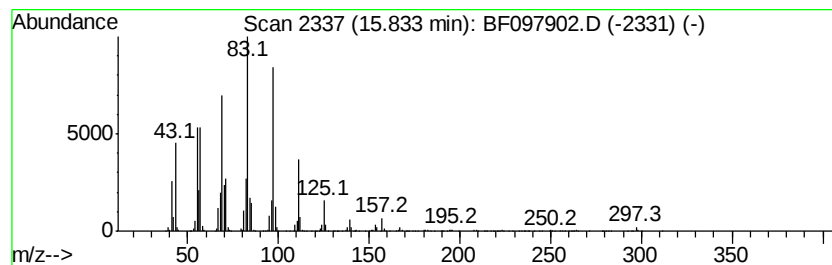
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Octacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	88.75 ng	3485660	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosanol	410	C28H58O	000557-61-9	70
2		1-Heptacosanol	396	C27H56O	002004-39-9	70
3		Cyclotetradecane	196	C14H28	000295-17-0	68
4		1-Docosene	308	C22H44	001599-67-3	64
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	62



Data Path : U:\HPCHEM1\BNA F\DATA\BF082117\
Data File : BF097902.D
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Misc :
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Instrument :
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ClientSampleId :
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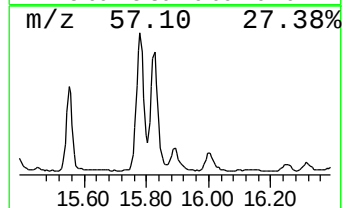
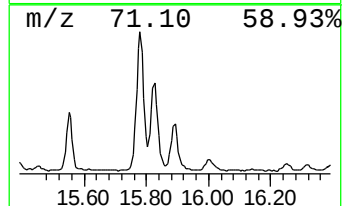
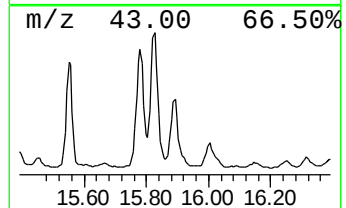
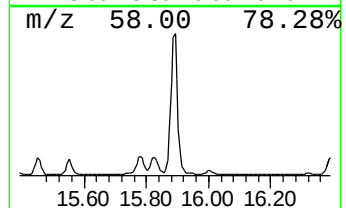
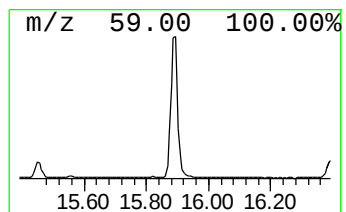
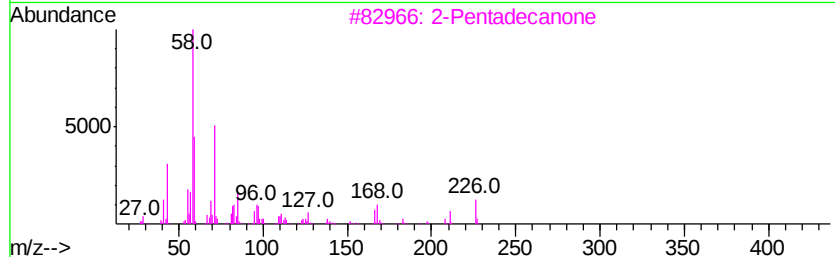
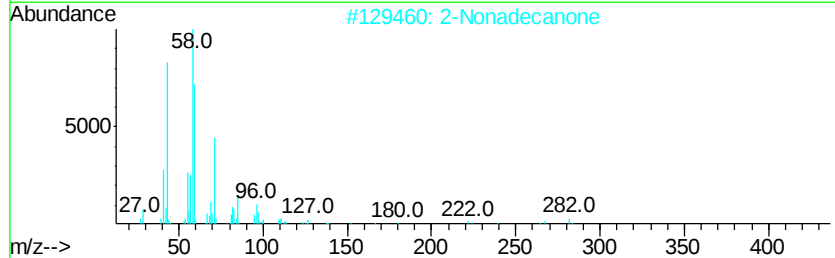
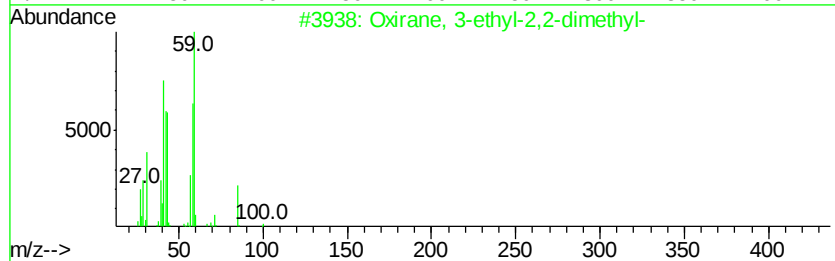
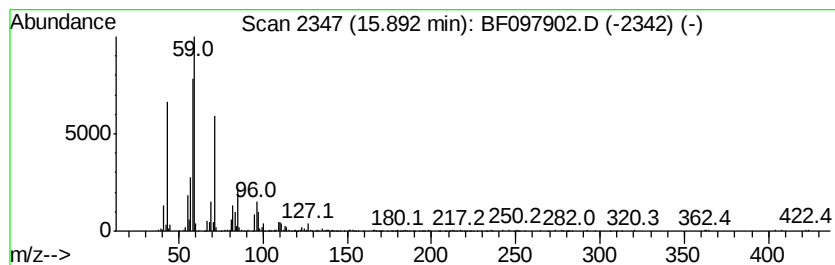
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Oxirane, 3-ethyl-2,2-dimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	32.69 ng	1284040	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, 3-ethyl-2,2-dimethyl-	100	C6H12O	001192-22-9	58
2		2-Nonadecanone	282	C19H38O	000629-66-3	50
3		2-Pentadecanone	226	C15H30O	002345-28-0	43
4		2-Tridecanone	198	C13H26O	000593-08-8	42
5		2-Pentacosanone	366	C25H50O	075207-54-4	38



Data Path : U:\HPCHEM1\BNA F\DATA\BF082117\
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Acq On : 21 Aug 2017 13:13
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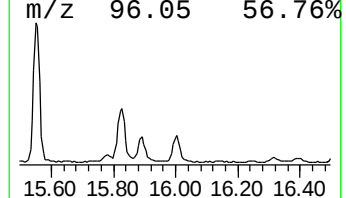
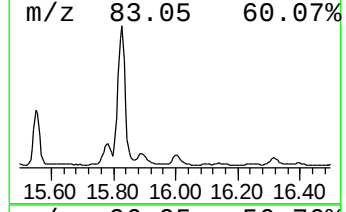
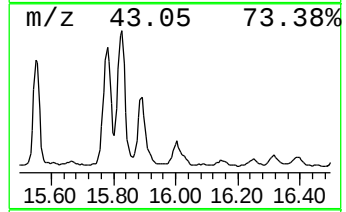
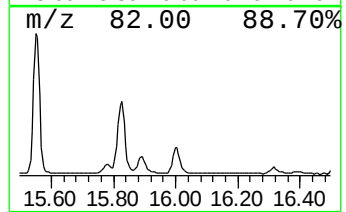
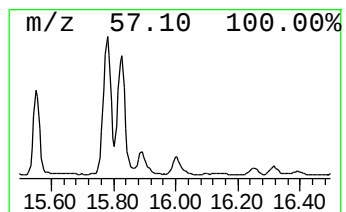
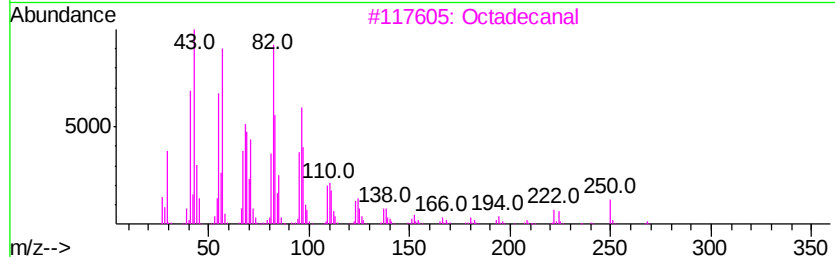
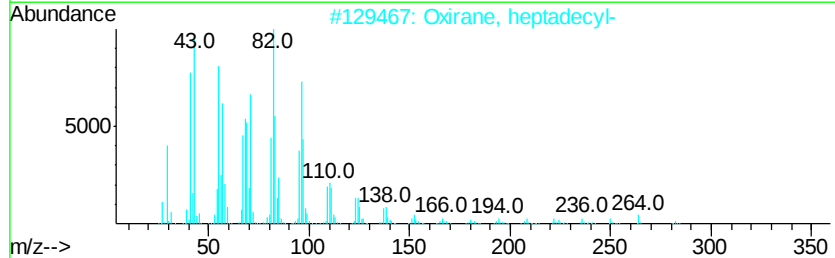
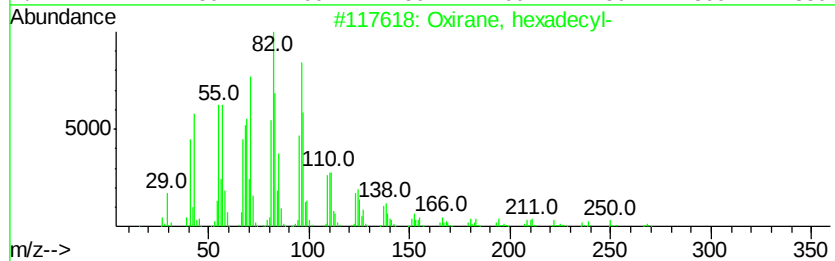
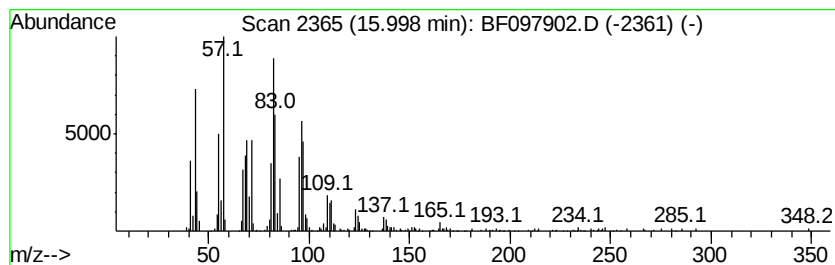
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Oxirane, hexadecyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	20.34 ng	798875	Perylene-d12	15.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
3		Octadecanal	268	C18H36O	000638-66-4	90
4		17-Octadecenal	266	C18H34O	056554-86-0	80
5		Hexadecanal	240	C16H32O	000629-80-1	72



Data Path : U:\HPCHEM1\BNA_F\DATA\BF082117\
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Acq On : 21 Aug 2017 13:13
Operator : SJ/JU
Sample : I4849-01
Misc :
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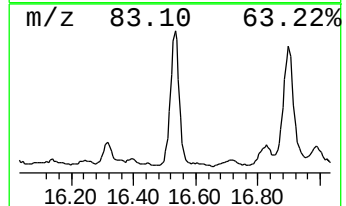
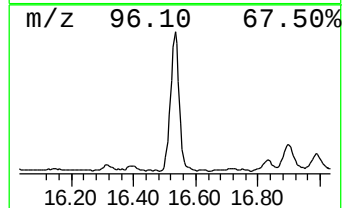
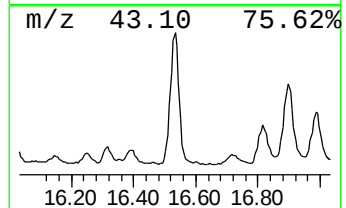
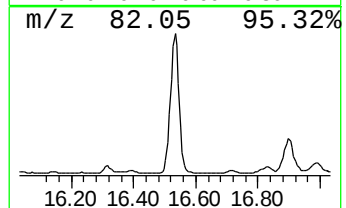
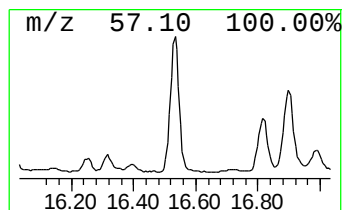
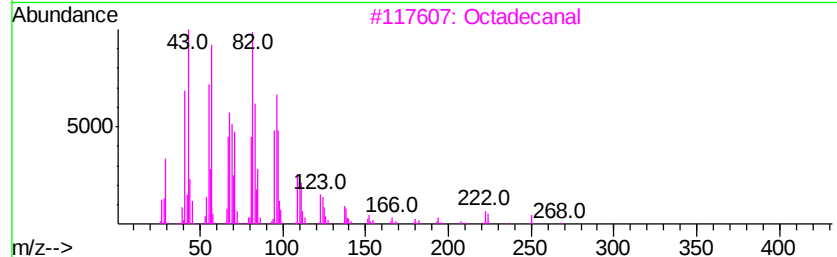
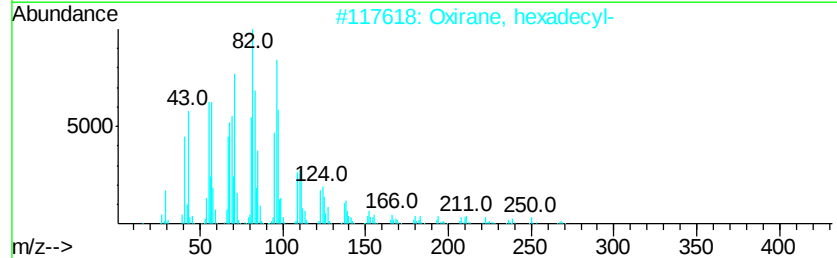
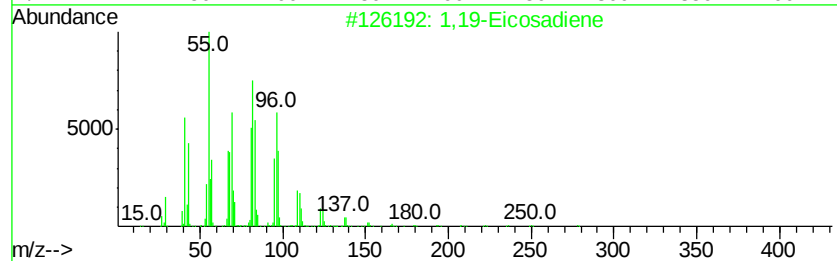
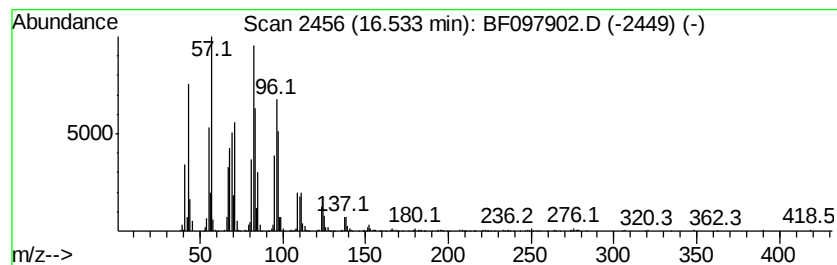
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 1,19-Eicosadiene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.53	63.79 ng	2505560	Perylene-d12	15.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	92
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3	Octadecanal	268	C18H36O	000638-66-4	91
4	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	86
5	Hexadecanal	240	C16H32O	000629-80-1	80



Data Path : U:\HPCHEM1\BNA_F\DATA\BF082117\
Data File : BF097902.D
Acq On : 21 Aug 2017 13:13
Operator : SJ/JU
Sample : I4849-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CAPTAINSCOVE-WC-002

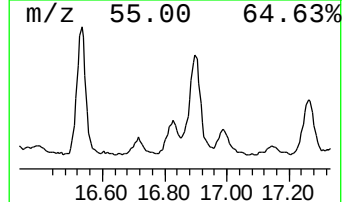
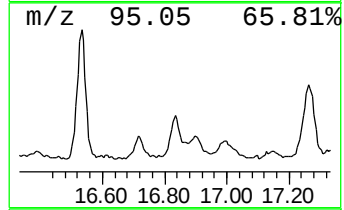
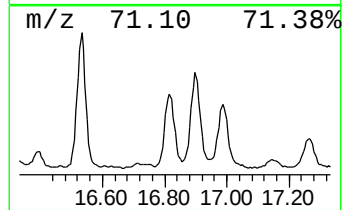
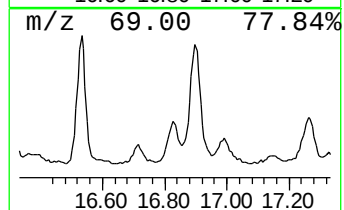
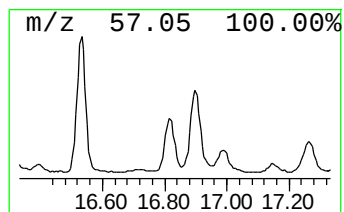
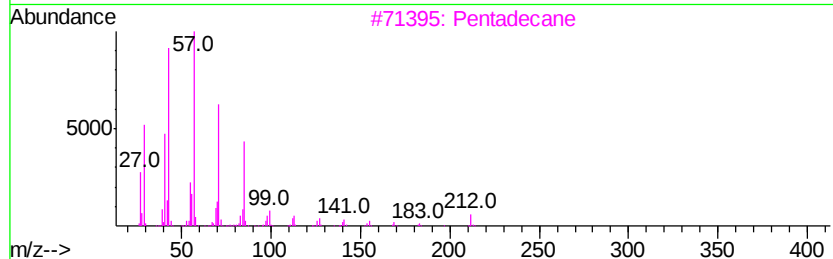
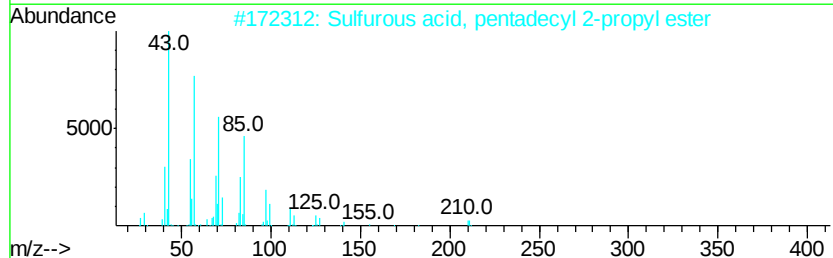
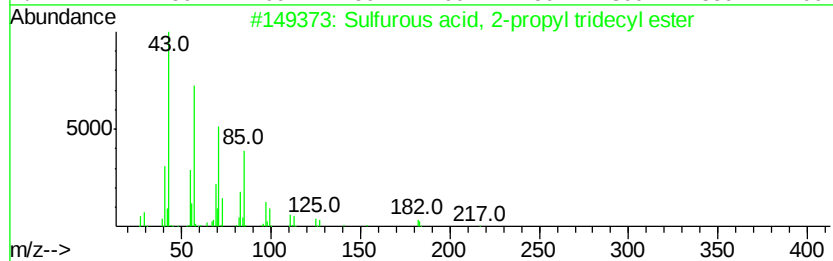
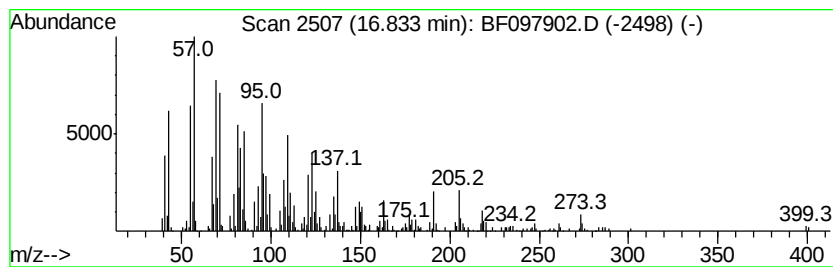
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Sulfurous acid, 2-propyl tr... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.83	26.54 ng	1042200	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, 2-propyl tridecyl...	306	C16H34O3S	1000309-12-4	60
2		Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	53
3		Pentadecane	212	C15H32	000629-62-9	52
4		Octadecane, 1-bromo-	332	C18H37Br	000112-89-0	52
5		1-Bromodocosane	388	C22H45Br	006938-66-5	49



Data Path : U:\HPCHEM1\BNA_F\DATA\BF082117\
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Acq On : 21 Aug 2017 13:13
Operator : SJ/JU
Sample : I4849-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

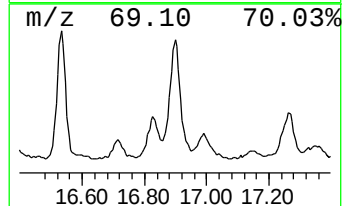
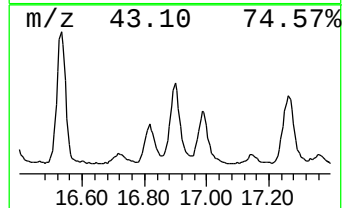
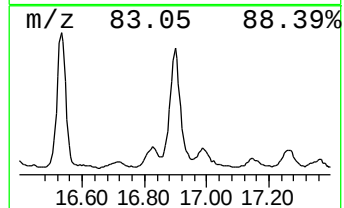
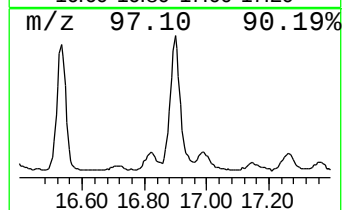
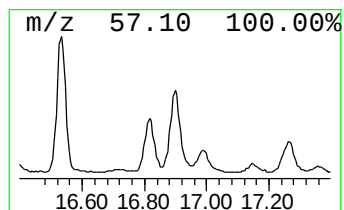
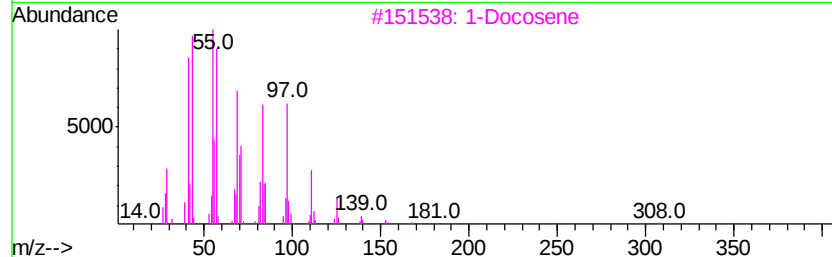
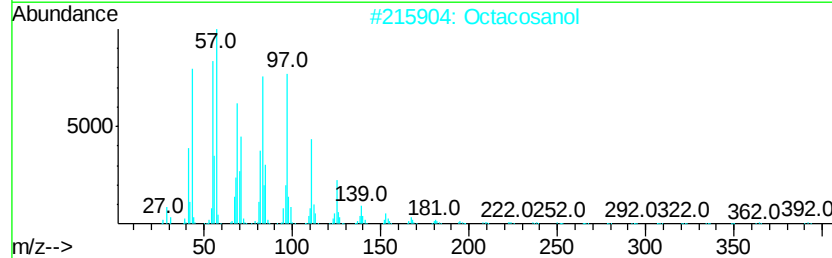
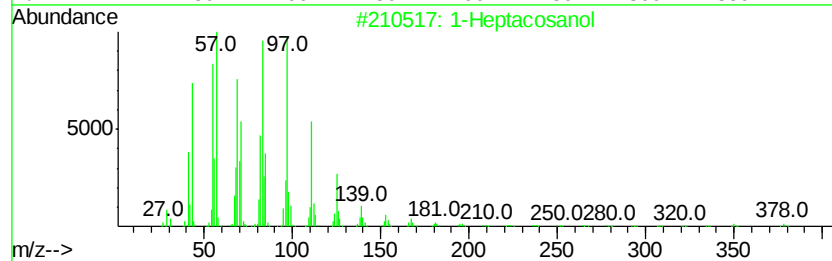
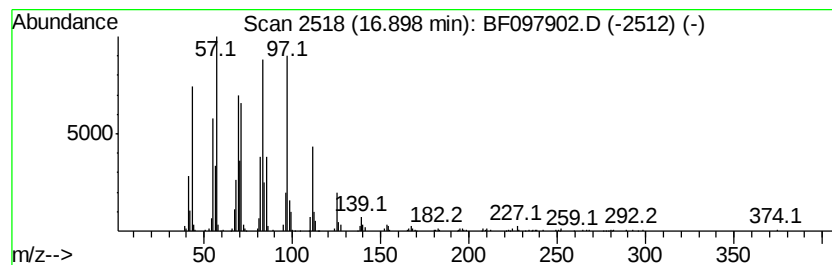
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 1-Heptacosanol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.90	50.73 ng	1992370	Perylene-d12	15.32
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Heptacosanol	396 C27H56O	002004-39-9 94
2		Octacosanol	410 C28H58O	000557-61-9 91
3		1-Docosene	308 C22H44	001599-67-3 91
4		17-Pentatriacontene	491 C35H70	006971-40-0 91
5		Pentafluoropropionic acid, hexad...	388 C19H33F5O2	006222-07-7 91



Data Path : U:\HPCHEM1\BNA_F\DATA\BF082117\
Data File : BF097902.D
Acq On : 21 Aug 2017 13:13
Operator : SJ/JU
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CAPTAINSCOVE-WC-002

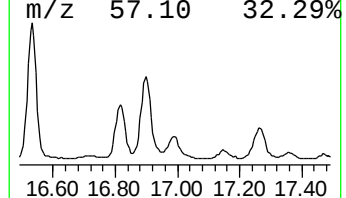
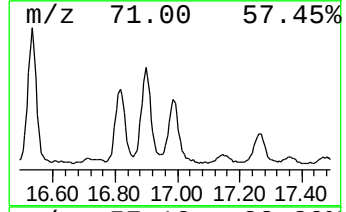
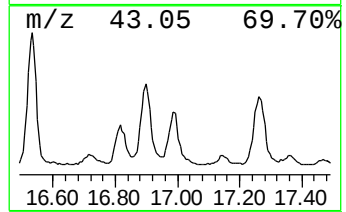
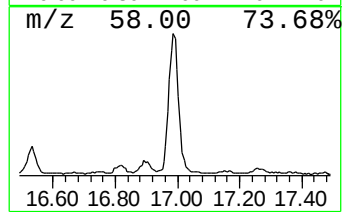
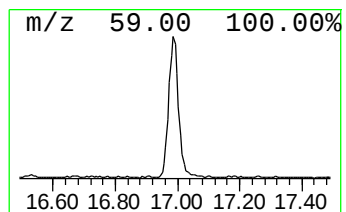
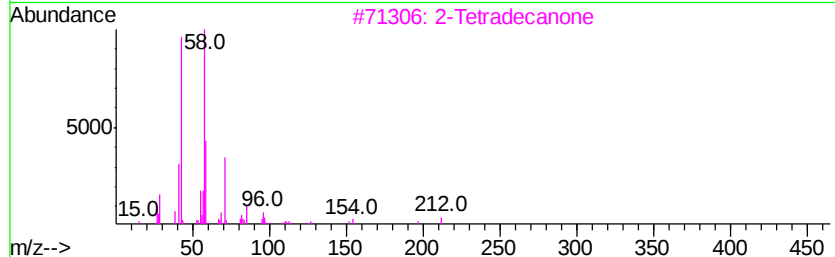
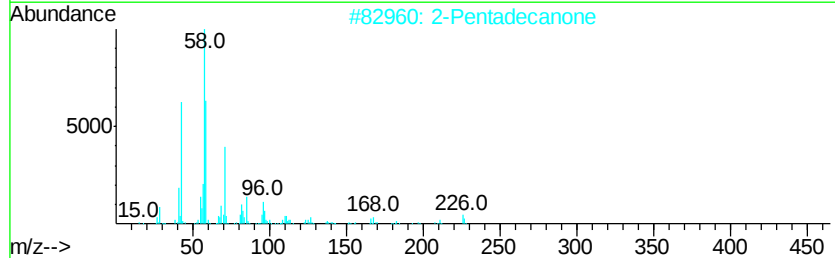
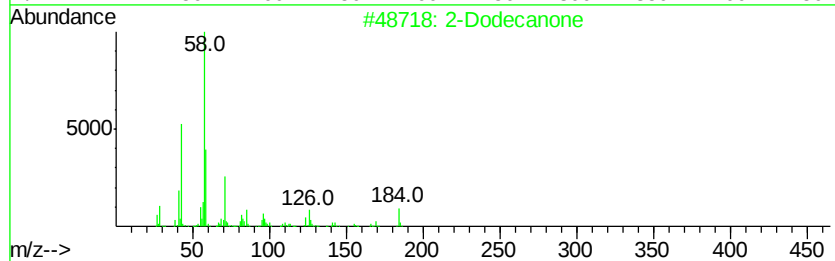
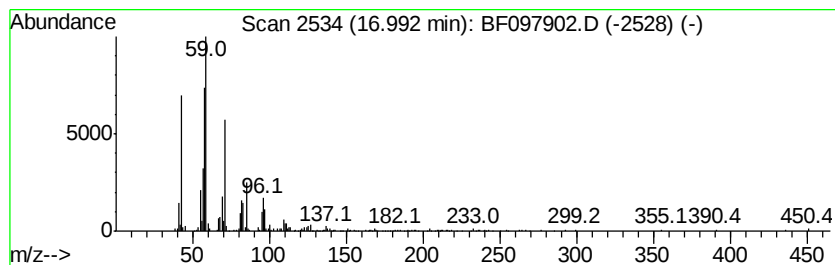
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 2-Dodecanone Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.99	23.78 ng	934036	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Dodecanone	184	C12H24O	006175-49-1	59
2		2-Pentadecanone	226	C15H30O	002345-28-0	59
3		2-Tetradecanone	212	C14H28O	002345-27-9	59
4		Oxirane, 3-ethyl-2,2-dimethyl-	100	C6H12O	001192-22-9	50
5		Oxirane, tetramethyl-	100	C6H12O	005076-20-0	43



Data Path : U:\HPCHEM1\BNA_F\DATA\BF082117\
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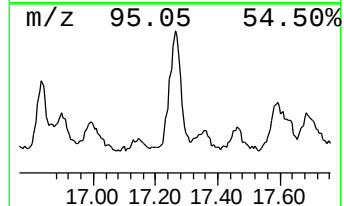
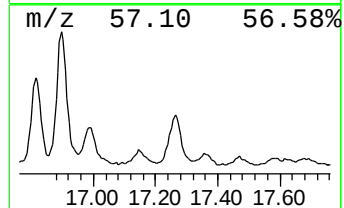
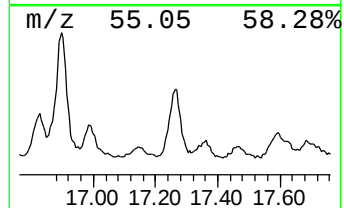
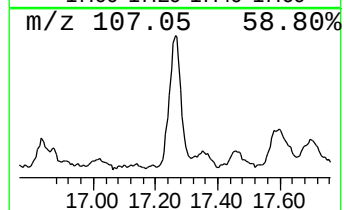
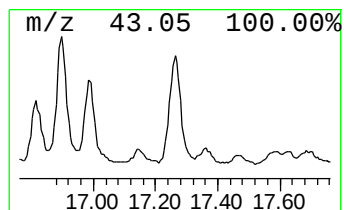
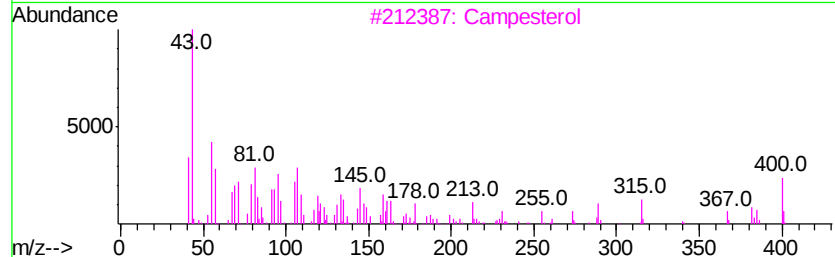
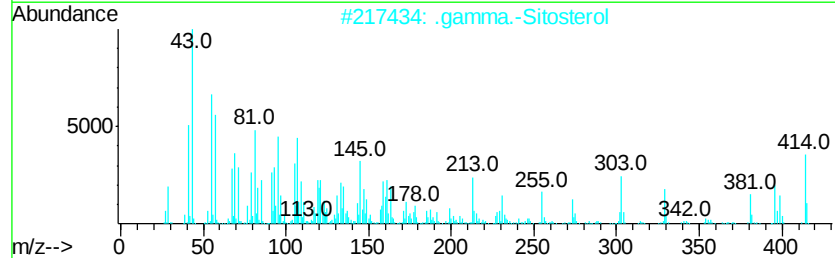
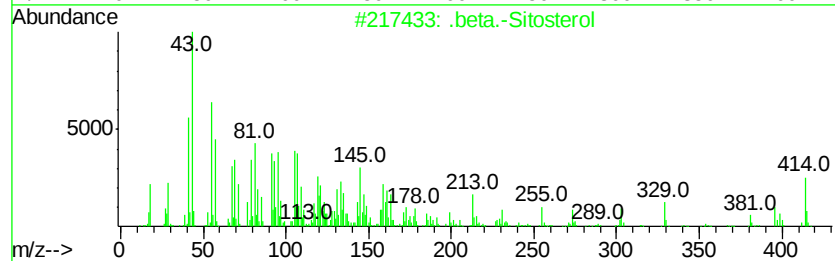
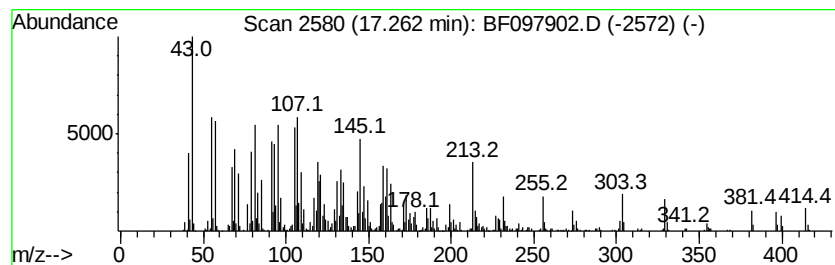
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 .beta.-Sitosterol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.26	59.53 ng	2338250	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-Sitosterol	414	C29H50O	000083-46-5	99
2		.gamma.-Sitosterol	414	C29H50O	000083-47-6	98
3		Campesterol	400	C28H48O	000474-62-4	58
4		Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	46
5		Ergost-7-en-3-ol, (3.beta.)-	400	C28H48O	026047-31-4	43



Data Path : U:\HPCHEM1\BNA F\DATA\BF082117\
Data File : BF097902.D
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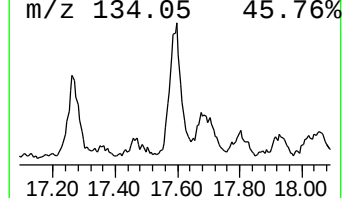
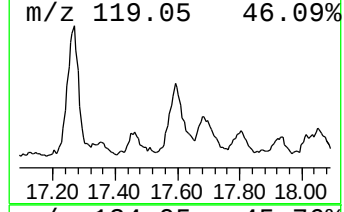
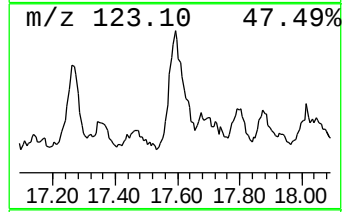
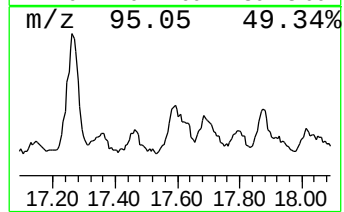
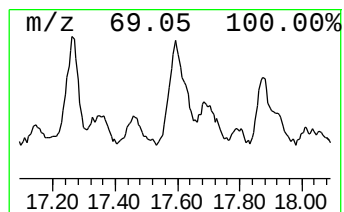
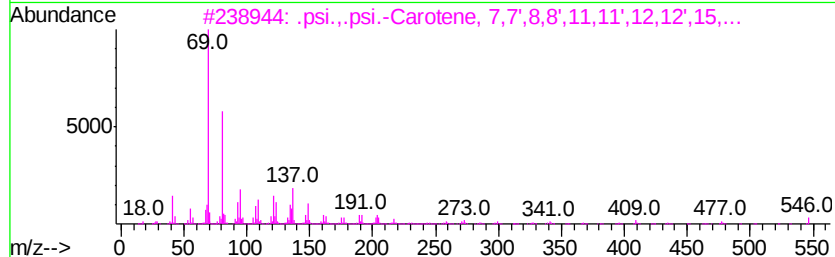
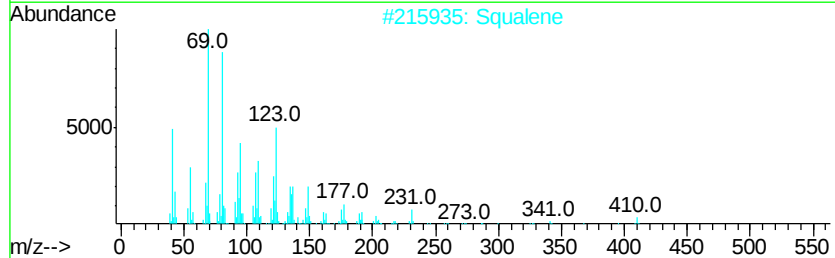
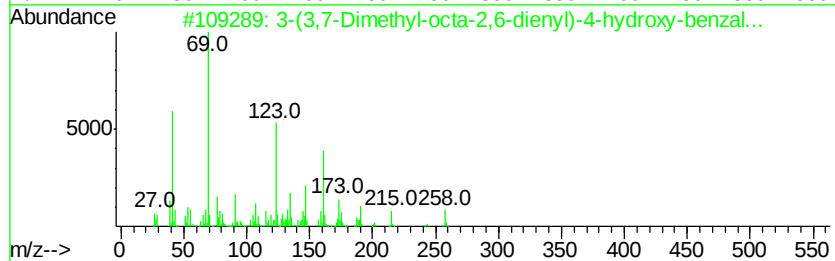
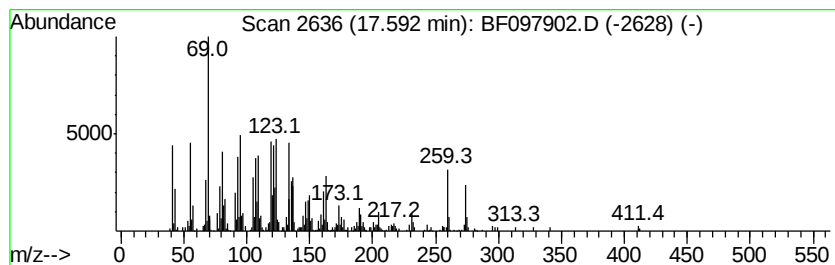
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 3-(3,7-Dimethyl-octa-2,6-di... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.59	26.64 ng	1046270	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-(3,7-Dimethyl-octa-2,6-dienvl)...	258	C17H22O2	1000192-28-0	92
2		Squalene	410	C30H50	000111-02-4	49
3		.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	25
4		(2,4,6-Trimethylcyclohexyl) meth...	156	C10H20O	013702-56-2	16
5		Farnesol, acetate	264	C17H28O2	1000352-67-2	12



Data Path : U:\HPCHEM1\BNA_F\DATA\BF082117\
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Acq On : 21 Aug 2017 13:13
Operator : SJ/JU
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Misc :
ALS Vial : 8 Sample Multiplier: 1

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CAPTAINSCOVE-WC-002

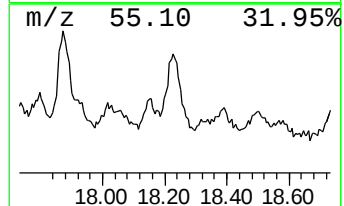
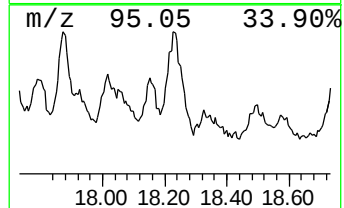
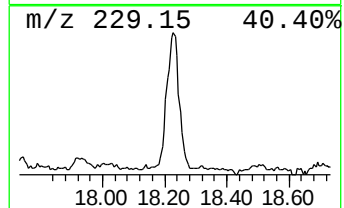
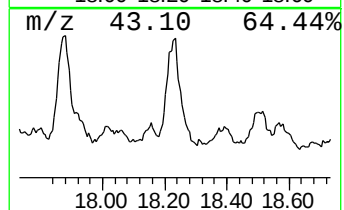
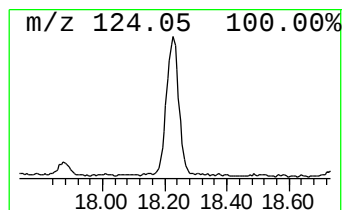
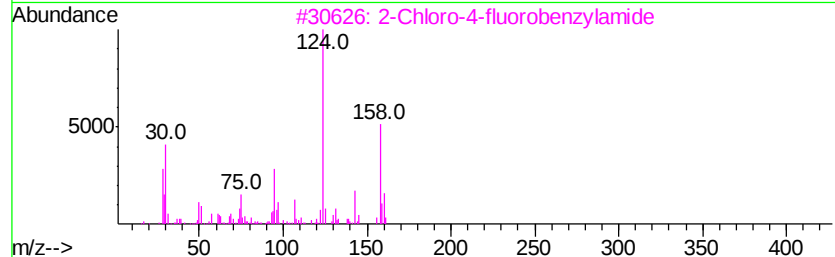
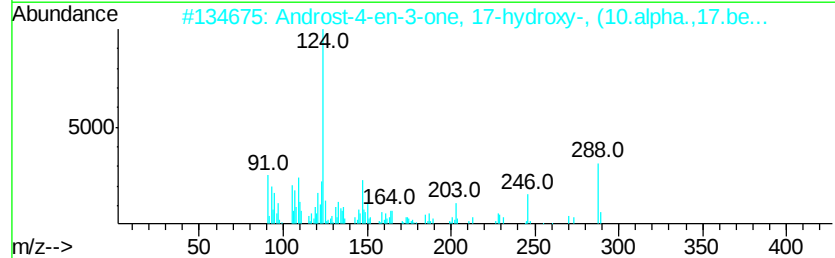
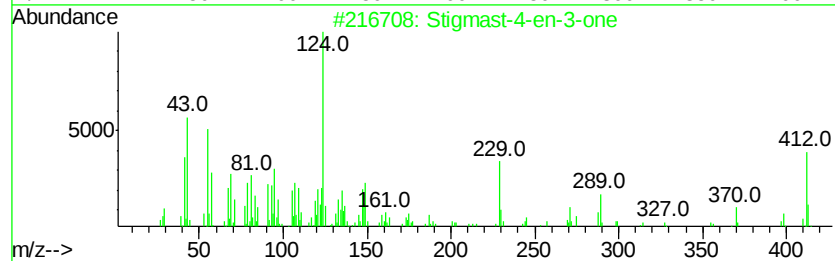
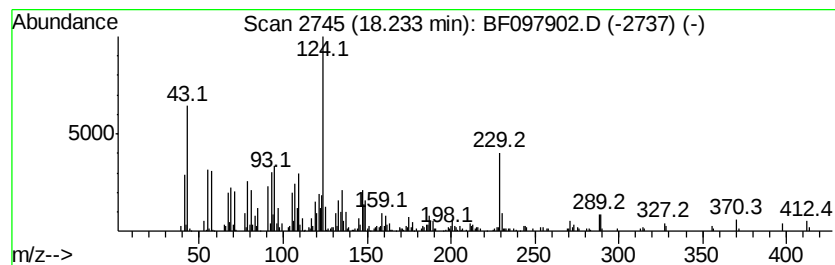
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 Stigmast-4-en-3-one Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.23	28.19 ng	1107330	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Stigmast-4-en-3-one	412	C29H48O	001058-61-3	94
2		Androst-4-en-3-one, 17-hydroxy-, ...	288	C19H28O2	000604-39-7	64
3		2-Chloro-4-fluorobenzylamide	159	C7H7ClFN	1000343-00-9	38
4		Pregn-4-en-3-one, 20,21-[(methyl...]	356	C22H33BO3	030882-65-6	38
5		Norfenefrine	153	C8H11NO2	000536-21-0	35



Data Path : U:\HPCHEM1\BNA F\DATA\BF082117\
Data File : BF097902.D
Acq On : 21 Aug 2017 13:13
Operator : SJ/JU
Sample : I4849-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CAPTAINSCOVE-WC-002

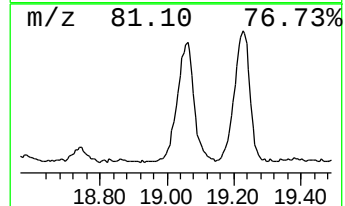
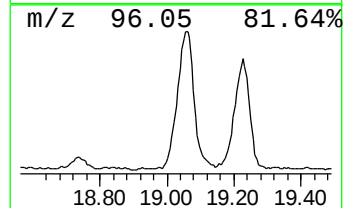
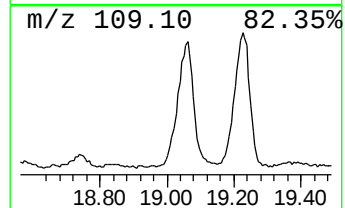
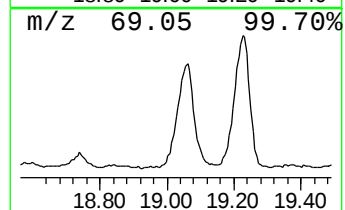
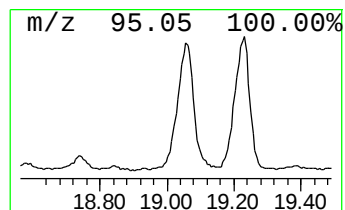
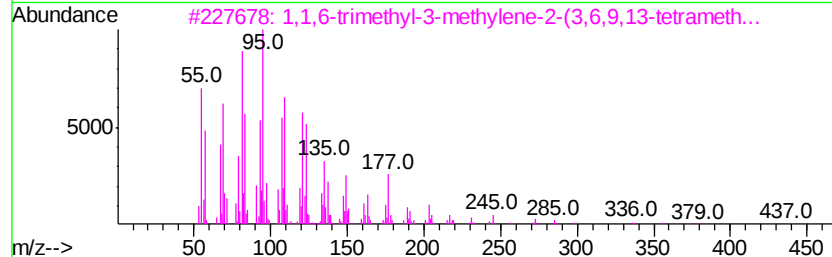
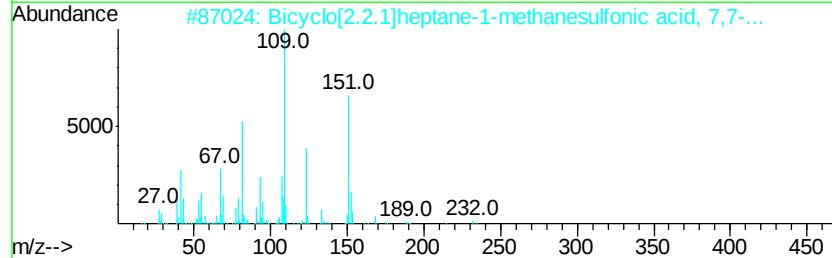
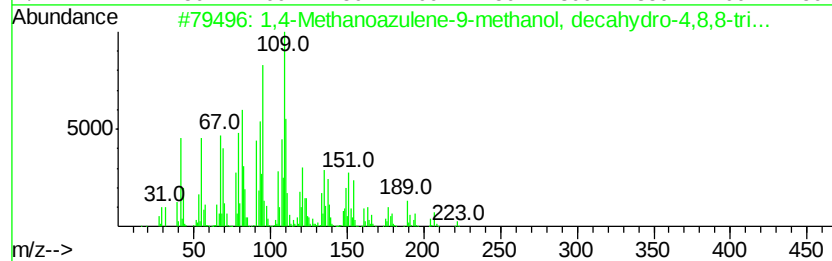
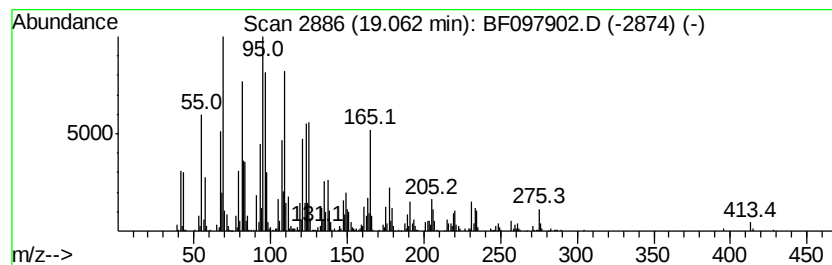
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 unknown19.06 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.06	75.91 ng	2981460	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Methanoazulene-9-methanol, d...	222	C15H26O	001139-17-9	49
2		Bicyclo[2.2.1]heptane-1-methanes...	232	C10H16O4S	005872-08-2	47
3		1,1,6-trimethyl-3-methylene-2-(3...	452	C33H56	1000373-94-5	45
4		1,1,6-trimethyl-3-methylene-2-(3...	442	C32H58	1000373-94-0	42
5		1-Formyl-2,2-dimethyl-3-trans-(3...	220	C15H24O	1000144-09-7	38



Data Path : U:\HPCHEM1\BNA F\DATA\BF082117\
Data File : BF097902.D
Acq On : 21 Aug 2017 13:13
Operator : SJ/JU
Sample : I4849-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CAPTAINSCOVE-WC-002

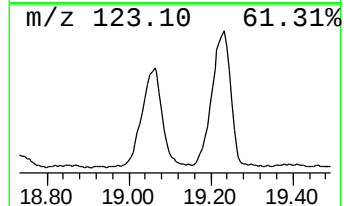
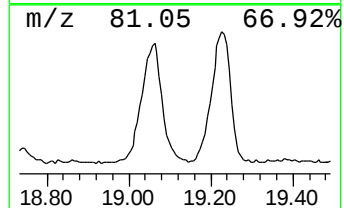
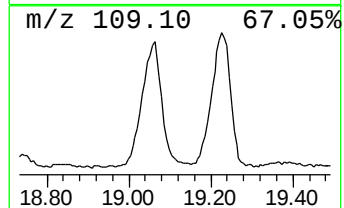
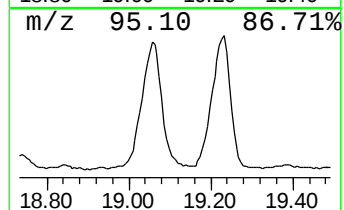
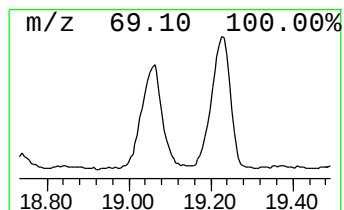
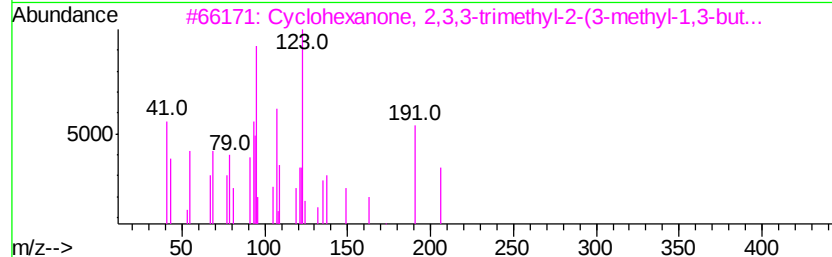
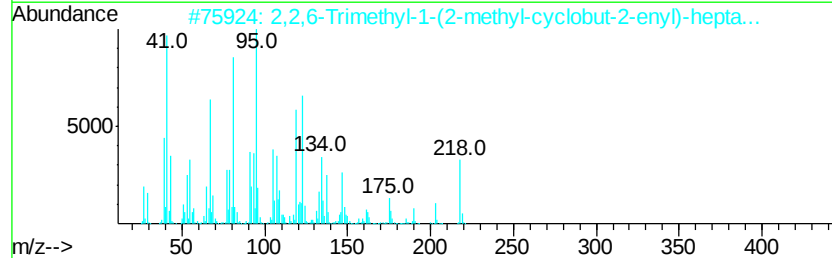
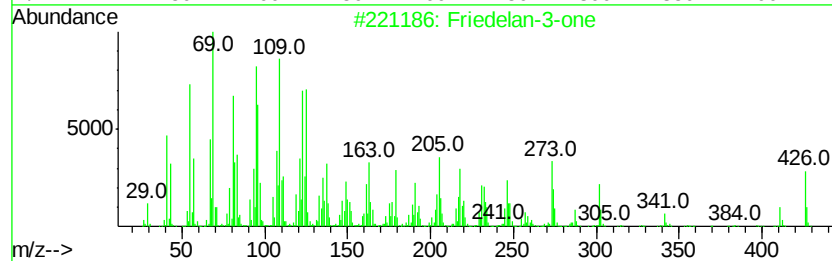
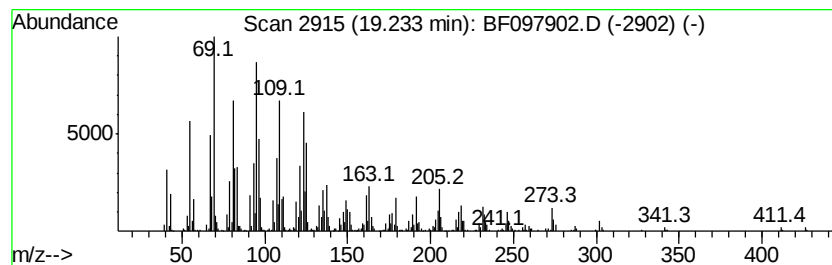
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 Friedelan-3-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.23	81.18 ng	3188600	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Friedelan-3-one	426	C30H50O	000559-74-0	95
2		2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	48
3		Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	35
4		Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	000473-55-2	27
5		Urea, N-[3-(1H-imidazol-1-yl)pro...	302	C17H26N4O	1000316-51-4	25



Data Path : U:\HPCHEM1\BNA_F\DATA\BF082117\
 Data File : BF097902.D
 Acq On : 21 Aug 2017 13:13
 Operator : SJ/JU
 Sample : I4849-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CAPTAINSCOVE-WC-002

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.52	6.52	84.1	ng	4030740	1	6.75	958914	20.0
3-Eicosene, (E)-	13.74	23.2	ng	1211860	5	13.89	1043340	20.0
Tritetracontane	14.38	53.2	ng	2775080	5	13.89	1043340	20.0
17-Octadecenal	14.82	42.7	ng	1676470	6	15.32	785518	20.0
Hexacosane	15.01	133.3	ng	5235370	6	15.32	785518	20.0
Octadecanal	15.55	55.1	ng	2165210	6	15.32	785518	20.0
Octacosane	15.78	47.7	ng	1873800	6	15.32	785518	20.0
Octacosanol	15.83	88.8	ng	3485660	6	15.32	785518	20.0
Oxirane, 3-ethyl-...	15.89	32.7	ng	1284040	6	15.32	785518	20.0
Oxirane, hexadecyl-	16.00	20.3	ng	798875	6	15.32	785518	20.0
1,19-Eicosadiene	16.53	63.8	ng	2505560	6	15.32	785518	20.0
Sulfurous acid, 2...	16.83	26.5	ng	1042200	6	15.32	785518	20.0
1-Heptacosanol	16.90	50.7	ng	1992370	6	15.32	785518	20.0
2-Dodecanone	16.99	23.8	ng	934036	6	15.32	785518	20.0
.beta.-Sitosterol	17.26	59.5	ng	2338250	6	15.32	785518	20.0
3-(3,7-Dimethyl-o...	17.59	26.6	ng	1046270	6	15.32	785518	20.0
Stigmast-4-en-3-one	18.23	28.2	ng	1107330	6	15.32	785518	20.0
unknown19.06	19.06	75.9	ng	2981460	6	15.32	785518	20.0
Friedelan-3-one	19.23	81.2	ng	3188600	6	15.32	785518	20.0