

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
 Data File : BF095577.D
 Acq On : 31 May 2017 22:16
 Operator : SJ/MA
 Sample : I3341-03
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NM14-COMP-0-6

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-BF050217.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	4.807	501	505	526	rBV	70047	176390	8.10%	0.898%
2	5.472	614	618	661	rBV	912517	1873333	86.05%	9.532%
3	7.107	892	896	910	rBV	1113113	1814334	83.34%	9.232%
4	7.213	910	914	926	rVB	1470801	2177101	100.00%	11.078%
5	7.554	968	972	983	rBV	442245	580429	26.66%	2.953%
6	7.789	1007	1012	1031	rBV	1276032	1664553	76.46%	8.470%
7	8.466	1122	1127	1143	rBV	876278	1291098	59.30%	6.570%
8	8.583	1143	1147	1157	rVB	120184	163854	7.53%	0.834%
9	9.583	1313	1317	1334	rBV	577425	807505	37.09%	4.109%
10	11.360	1613	1619	1637	rBV	1404552	1729123	79.42%	8.798%
11	12.048	1732	1736	1748	rVB	228880	286139	13.14%	1.456%
12	12.407	1792	1797	1806	rBV2	713186	949235	43.60%	4.830%
13	13.254	1935	1941	1947	rBV	40112	48731	2.24%	0.248%
14	13.707	2013	2018	2031	rBV	721829	1016394	46.69%	5.172%
15	14.024	2067	2072	2075	rBV2	47459	58602	2.69%	0.298%
16	14.759	2190	2197	2201	rBV	18984	25112	1.15%	0.128%
17	14.807	2201	2205	2210	rVV	450303	591726	27.18%	3.011%
18	14.848	2210	2212	2219	rVB	82211	109373	5.02%	0.557%
19	15.606	2335	2341	2345	rBV3	13992	23093	1.06%	0.118%
20	15.795	2370	2373	2382	rVB2	99682	131861	6.06%	0.671%
21	16.612	2508	2512	2522	rBV	182769	217142	9.97%	1.105%
22	16.695	2522	2526	2533	rVV	43899	45035	2.07%	0.229%
23	16.912	2554	2563	2569	rBV	190284	251359	11.55%	1.279%
24	17.153	2600	2604	2610	rBV	1001395	1057327	48.57%	5.380%
25	17.383	2640	2643	2648	rVB2	17970	23682	1.09%	0.121%
26	17.518	2662	2666	2669	rBV4	19365	27466	1.26%	0.140%
27	17.853	2720	2723	2727	rVB2	17721	21781	1.00%	0.111%
28	17.995	2744	2747	2750	rVB	23041	22379	1.03%	0.114%
29	18.406	2811	2817	2827	rBV3	68497	132846	6.10%	0.676%
30	18.506	2828	2834	2837	rVV2	543087	713701	32.78%	3.632%
31	18.542	2837	2840	2847	rVB3	74572	135032	6.20%	0.687%
32	18.812	2881	2886	2890	rBV3	34767	45005	2.07%	0.229%
33	19.200	2948	2952	2959	rVB4	41246	52830	2.43%	0.269%
34	19.630	3022	3025	3030	rVB2	23858	32683	1.50%	0.166%

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

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	19.777	3046	3050	3053	rBV	105158	137237	6.30%	0.698%
36	19.889	3066	3069	3072	rBV	21679	24970	1.15%	0.127%
37	19.924	3072	3075	3077	rBV	34840	38124	1.75%	0.194%
38	20.065	3096	3099	3103	rBV	70714	75103	3.45%	0.382%
39	20.124	3106	3109	3113	rVV	90785	98711	4.53%	0.502%
40	20.177	3114	3118	3128	rVV	473537	585588	26.90%	2.980%
41	20.265	3131	3133	3139	rVB6	15471	23625	1.09%	0.120%
42	20.618	3189	3193	3197	rBV	104980	137678	6.32%	0.701%
43	20.906	3238	3242	3249	rVB8	42684	87577	4.02%	0.446%
44	21.436	3328	3332	3335	rBV2	36806	61041	2.80%	0.311%
45	21.471	3336	3338	3342	rVV4	19883	30400	1.40%	0.155%
46	21.800	3389	3394	3397	rBV2	32012	56545	2.60%	0.288%

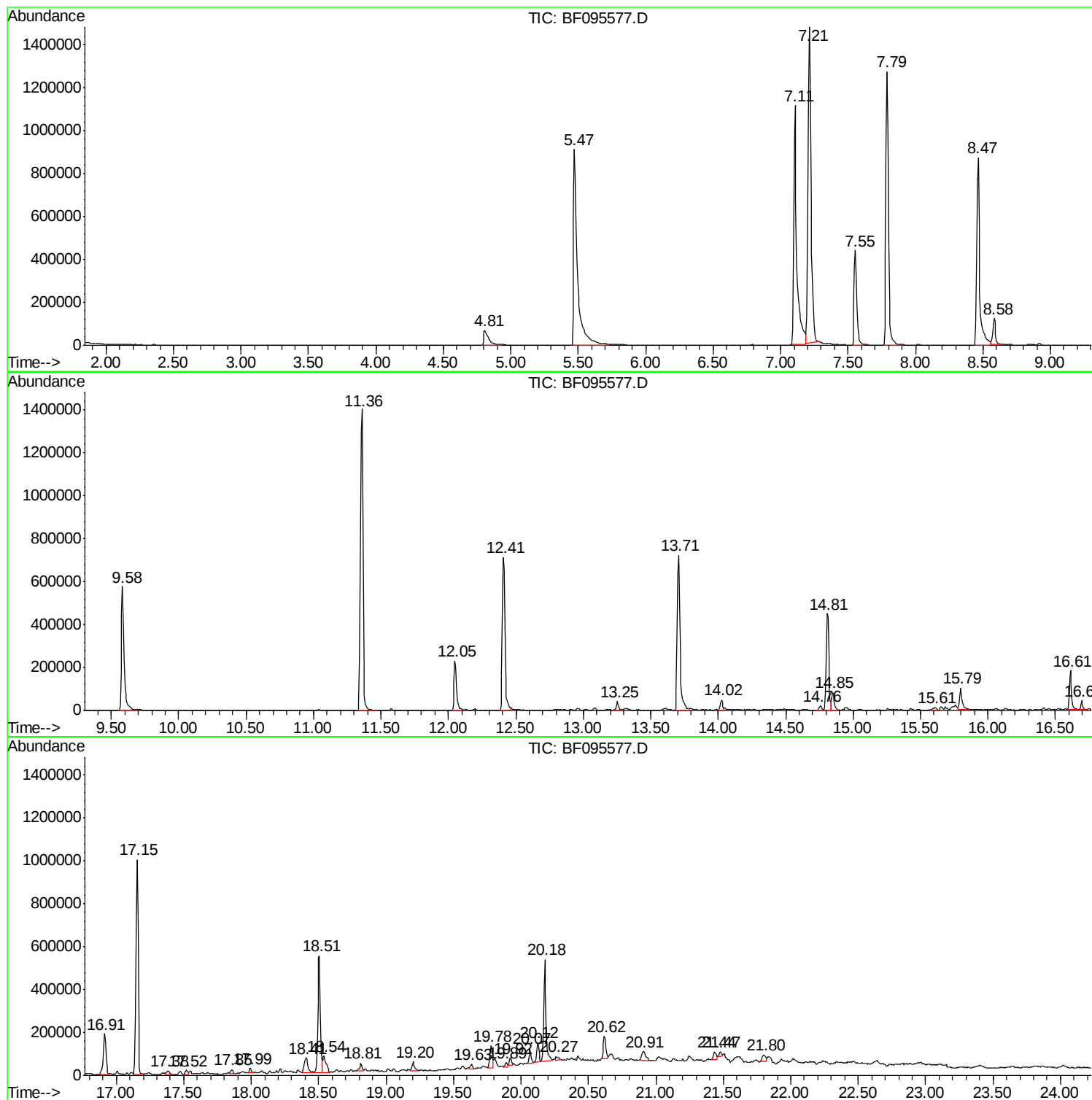
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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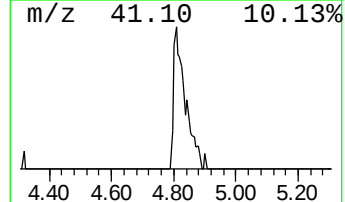
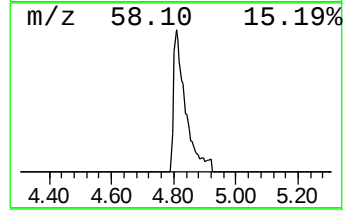
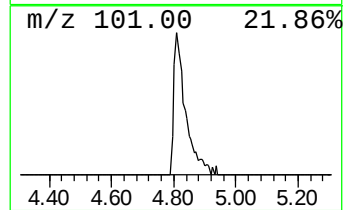
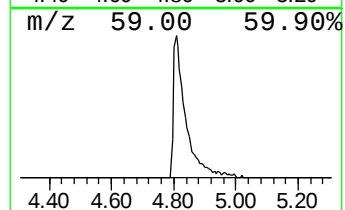
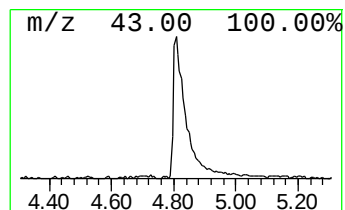
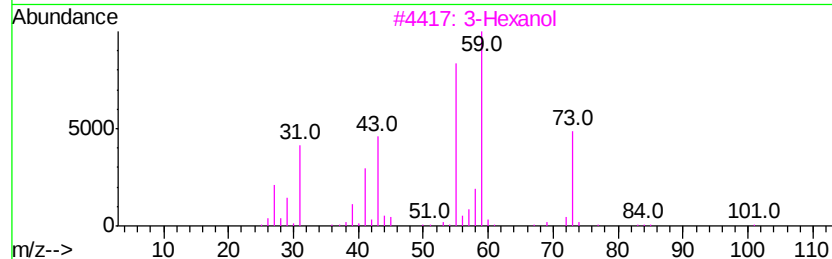
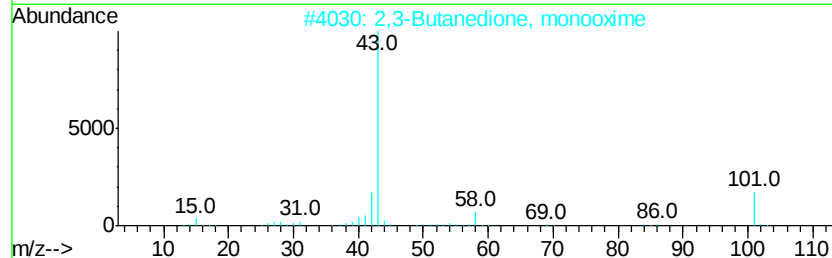
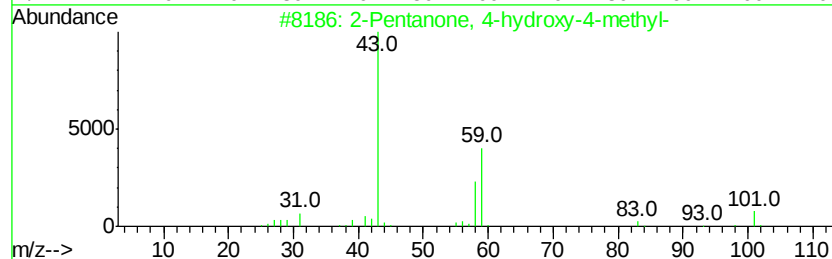
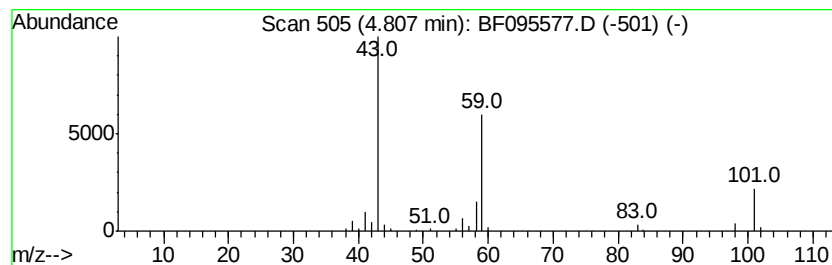
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	6.08 ng	176390	1,4-Dichlorobenzene-d4	7.55

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3			3-Hexanol	102	C6H14O	000623-37-0	28
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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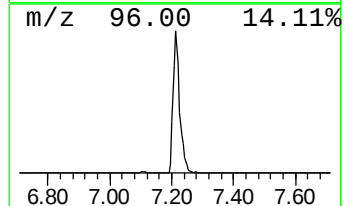
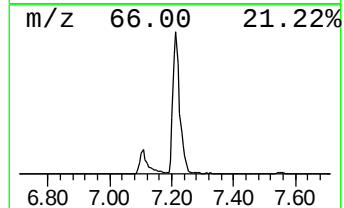
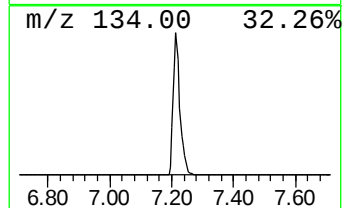
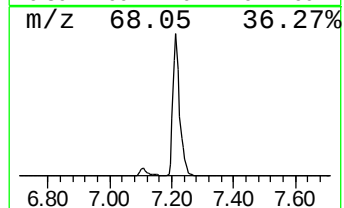
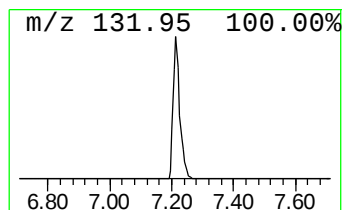
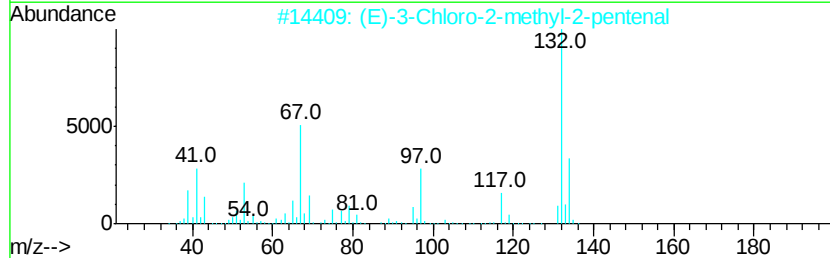
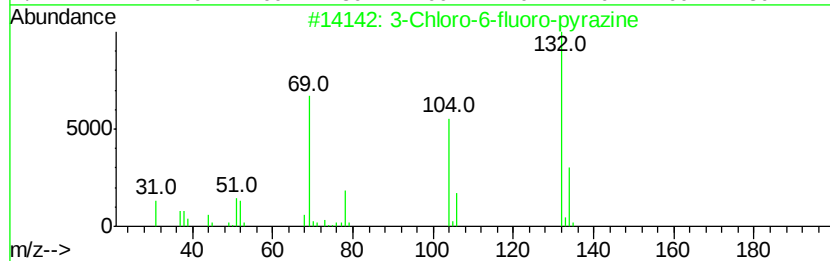
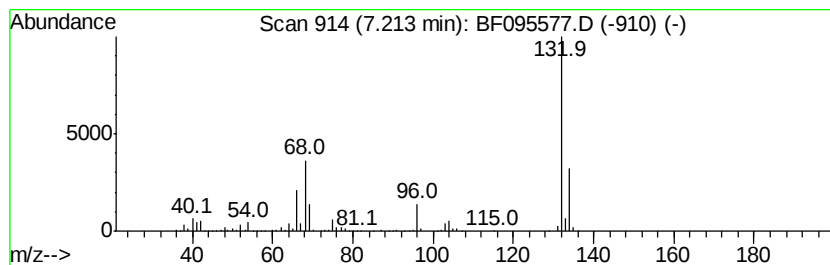
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown7.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	75.02 ng	2177100	1,4-Dichlorobenzene-d4	7.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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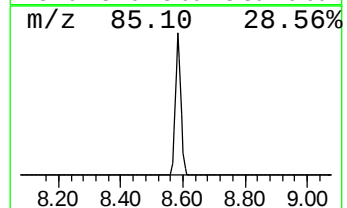
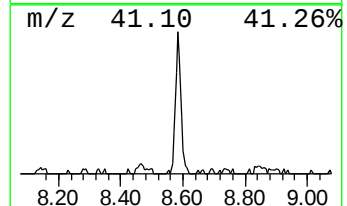
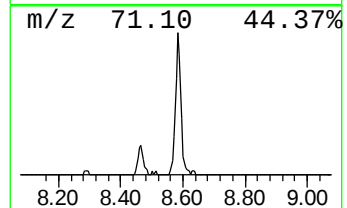
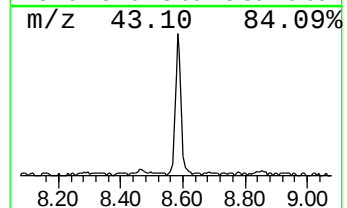
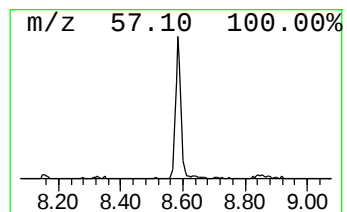
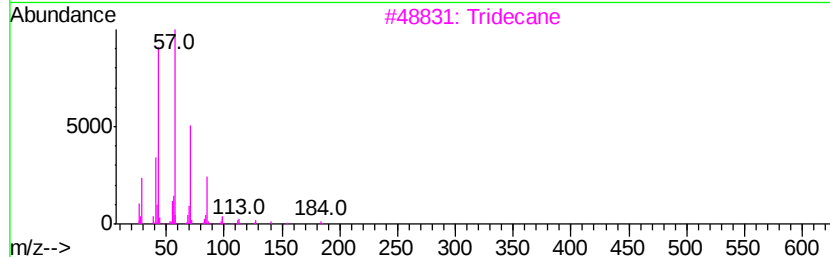
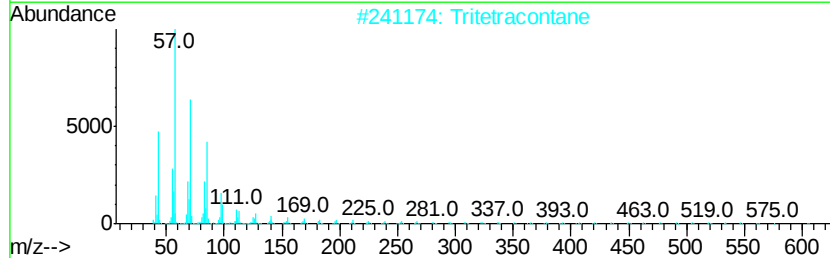
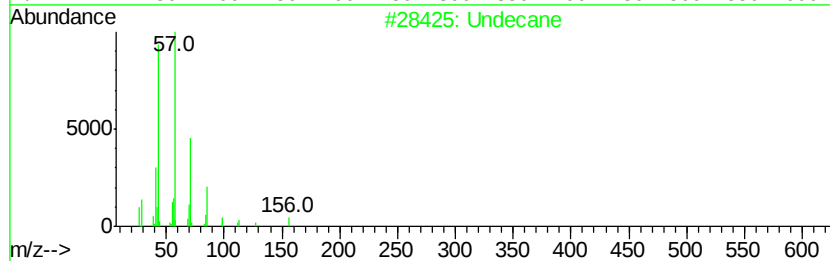
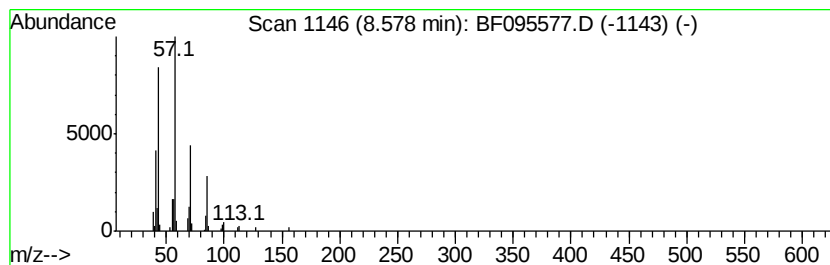
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Undecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.58	4.06 ng	163854	Napthalene-d8	9.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecane	156	C11H24	001120-21-4	91
2		Tritetracontane	605	C43H88	007098-21-7	83
3		Tridecane	184	C13H28	000629-50-5	80
4		Hexadecane	226	C16H34	000544-76-3	78
5		Tetradecane	198	C14H30	000629-59-4	78



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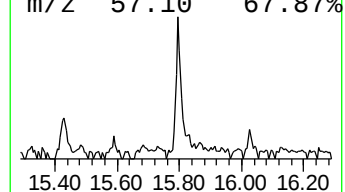
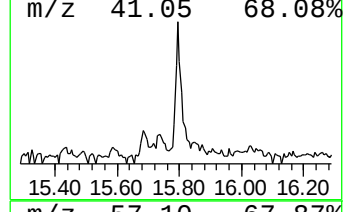
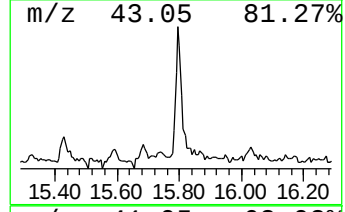
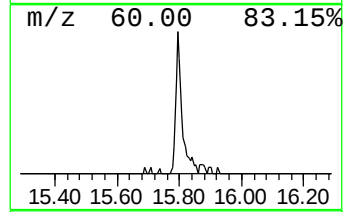
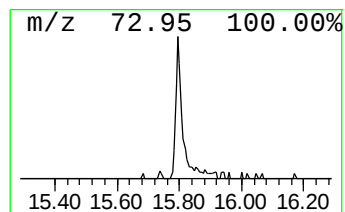
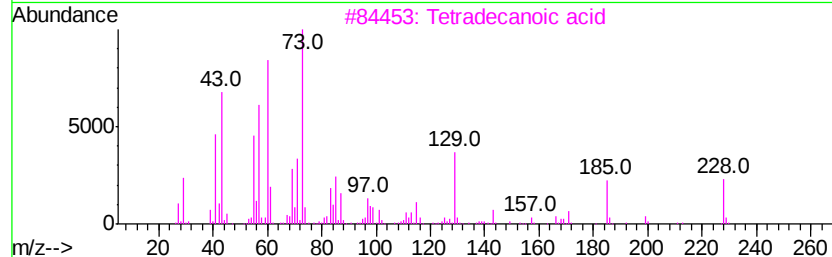
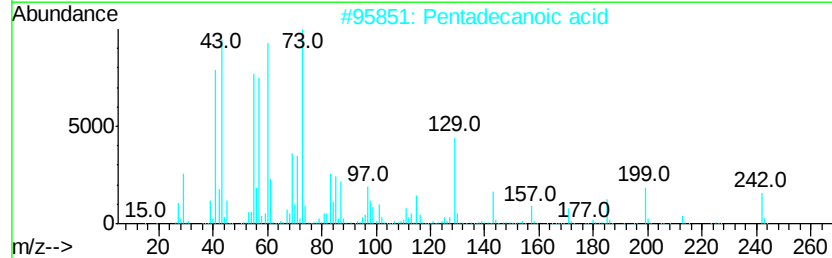
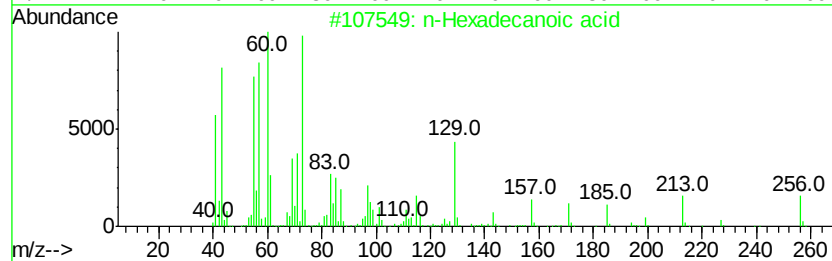
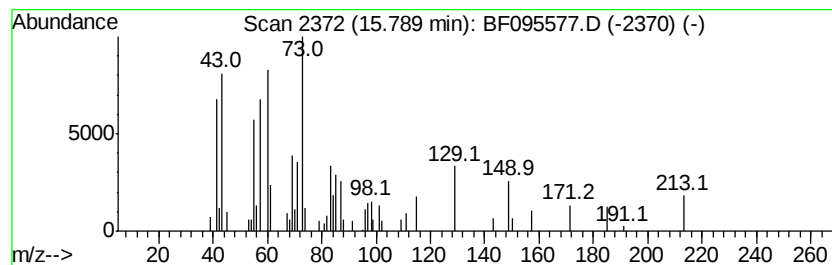
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	4.46 ng	131861	Phenanthrene-d10	14.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4		Tridecanoic acid	214	C13H26O2	000638-53-9	58
5		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58



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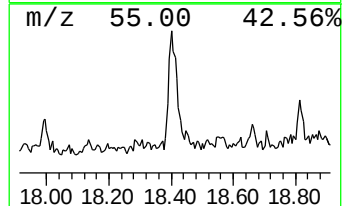
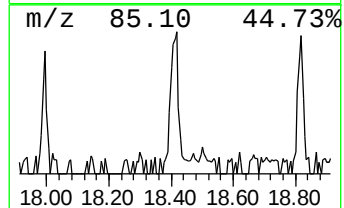
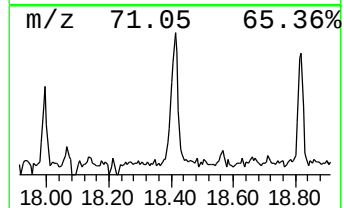
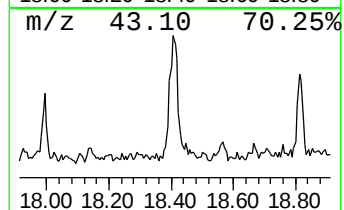
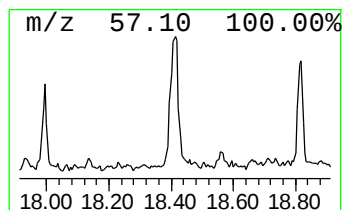
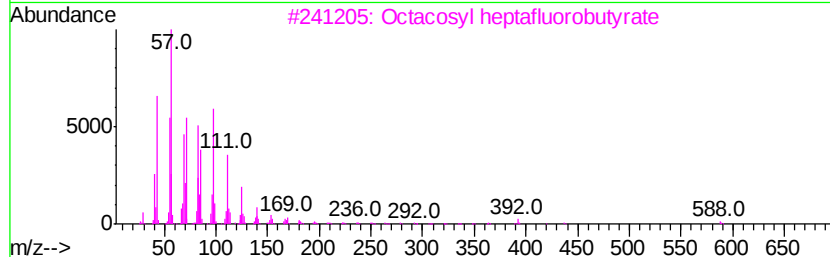
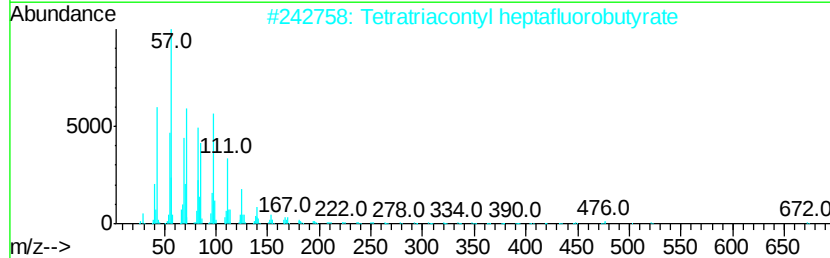
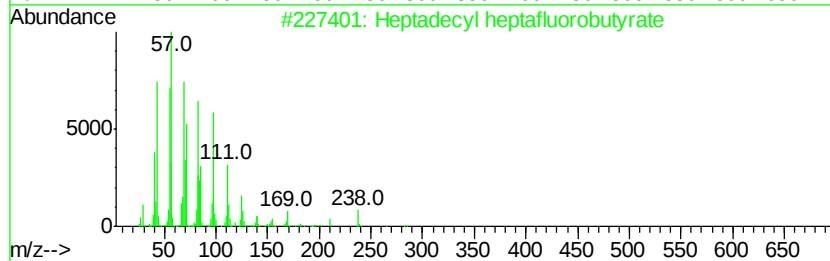
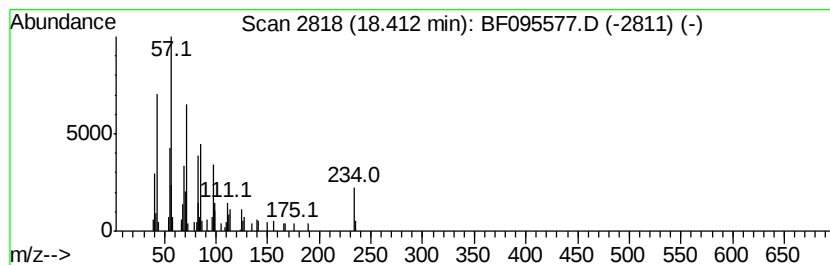
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.41	3.72 ng	132846	Chrysene-d12	18.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	92
2		Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	70
3		Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	70
4		Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	70
5		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	62



Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095577.D
Acq On : 31 May 2017 22:16
Operator : SJ/MA
Sample : I3341-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

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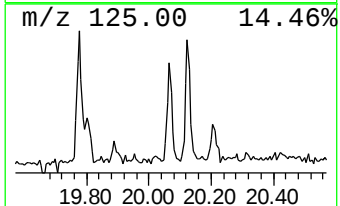
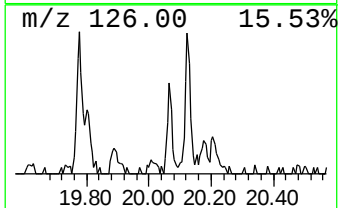
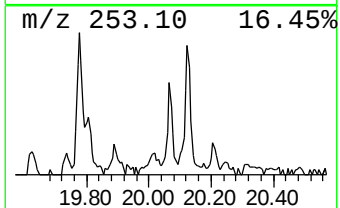
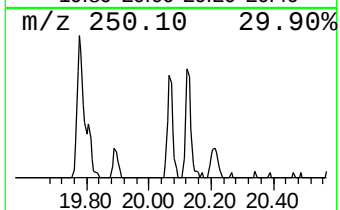
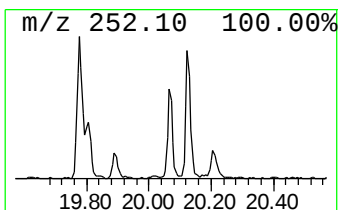
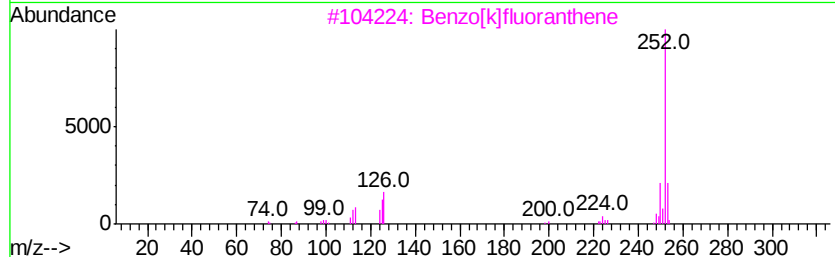
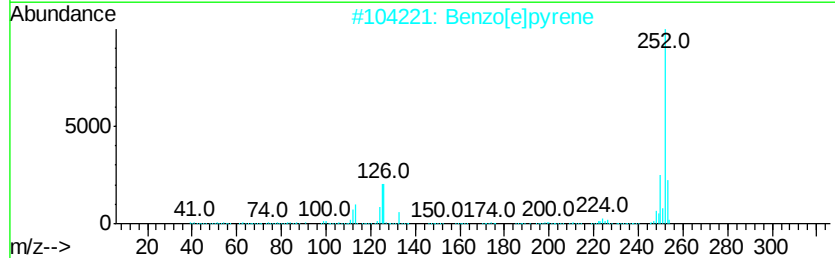
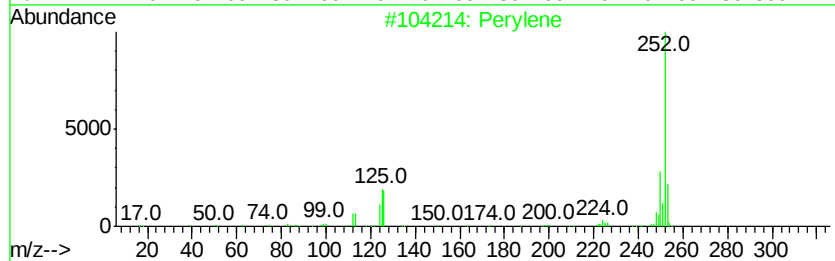
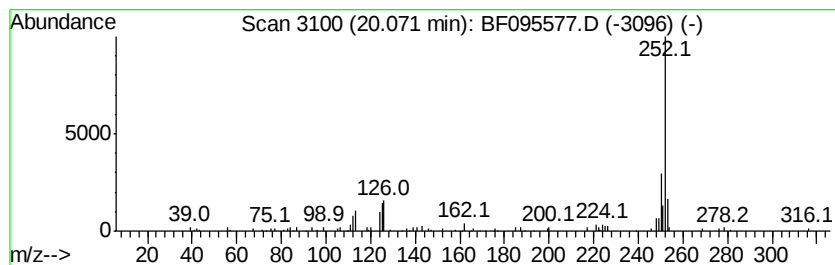
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Perylene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.07	2.57 ng	75103	Perylene-d12	20.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Perylene	252	C20H12	000198-55-0	98
2		Benzo[e]pyrene	252	C20H12	000192-97-2	97
3		Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
4		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	93
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	93



Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095577.D
Acq On : 31 May 2017 22:16
Operator : SJ/MA
Sample : I3341-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM14-COMP-0-6

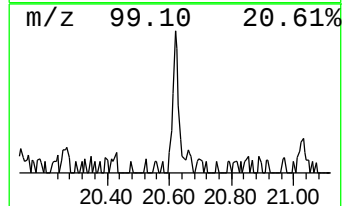
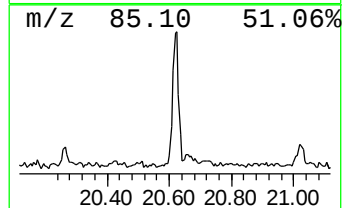
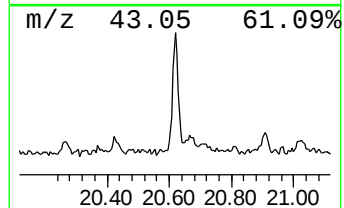
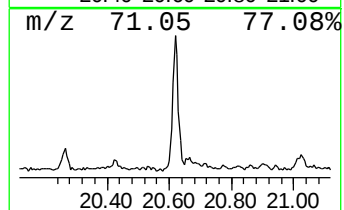
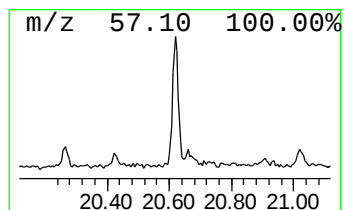
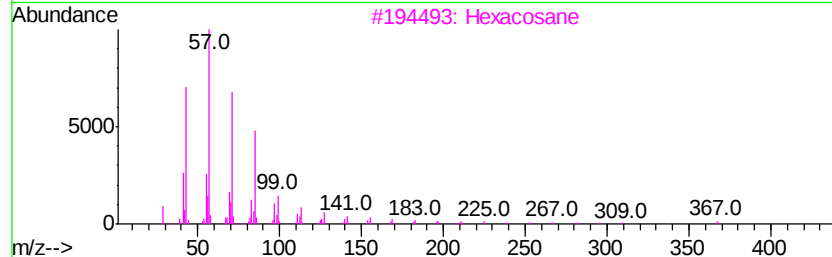
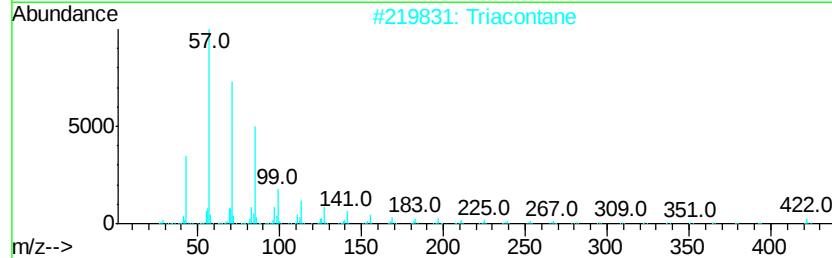
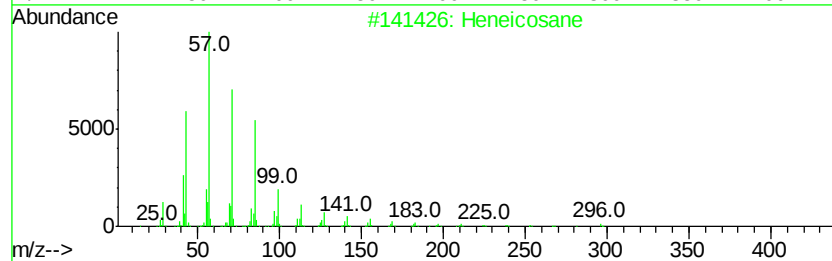
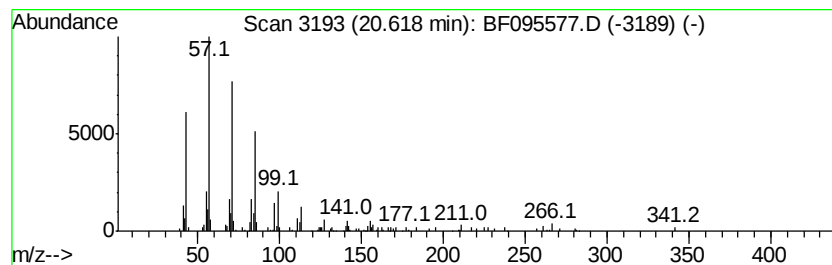
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.62	4.70 ng	137678	Perylene-d12	20.18

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Triacontane		422	C30H62	000638-68-6	90
3	Hexacosane		366	C26H54	000630-01-3	90
4	Hexadecane		226	C16H34	000544-76-3	86
5	Docosane, 11-decyl-		451	C32H66	055401-55-3	86



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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM14-COMP-0-6

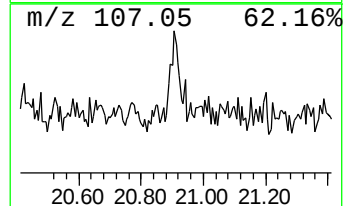
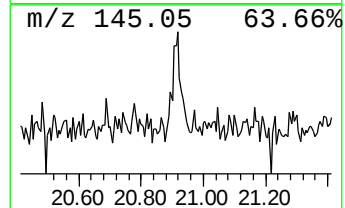
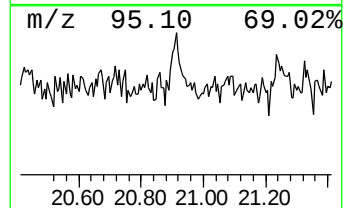
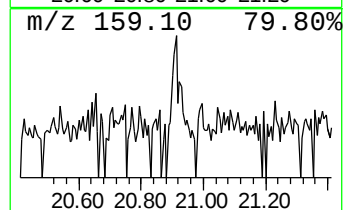
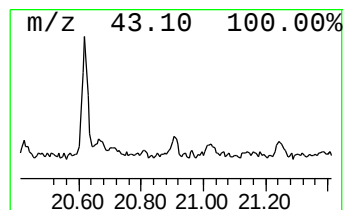
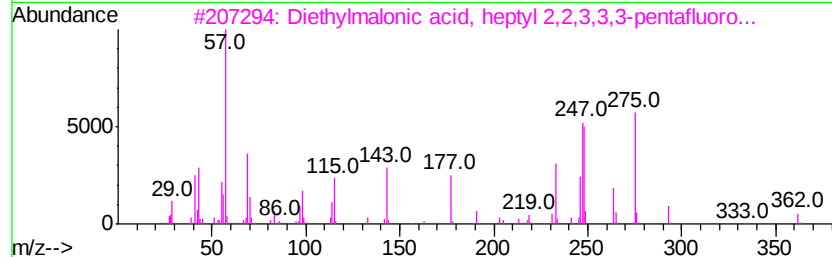
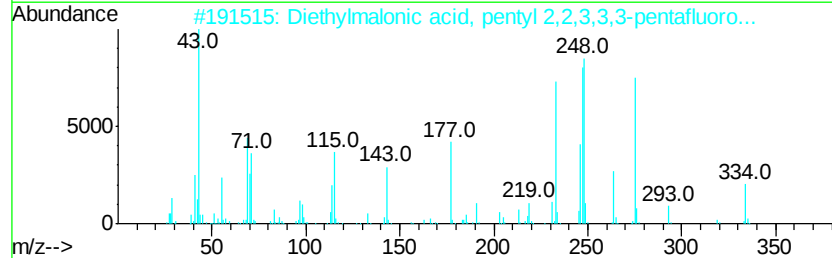
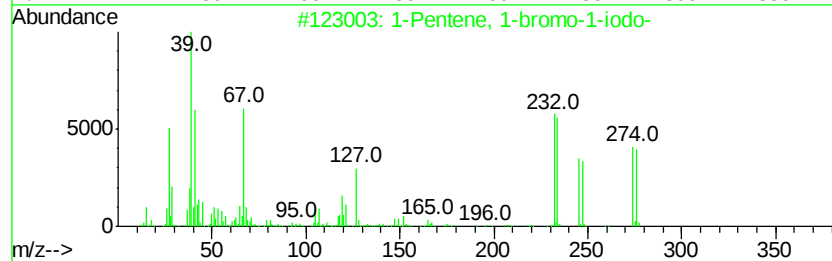
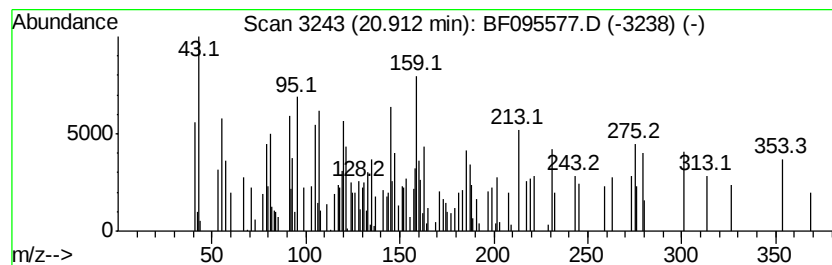
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown20.91 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.91	2.99 ng	87577	Perylene-d12	20.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Pentene, 1-bromo-1-iodo-	274	C5H8BrI	055683-02-8	10
2		Diethylmalonic acid, pentyl 2,2,...	362	C15H23F5O4	1000370-84-1	10
3		Diethylmalonic acid, heptyl 2,2,...	390	C17H27F5O4	1000370-84-4	9
4		Diethylmalonic acid, hexyl 2,2,3...	376	C16H25F5O4	1000370-84-3	9
5		16-Allopregnen-3.beta.-ol-20-one	316	C21H32O2	000566-61-0	9



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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM14-COMP-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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
2-Pentanone, 4-hy...	4.81	6.1 ng		176390	1	7.55	580429	20.0
unknown7.21	7.21	75.0 ng		2177100	1	7.55	580429	20.0
Undecane	8.58	4.1 ng		163854	2	9.58	807505	20.0
n-Hexadecanoic acid	15.79	4.5 ng		131861	4	14.81	591726	20.0
Heptadecyl hepta...	18.41	3.7 ng		132846	5	18.51	713701	20.0
Perylene	20.07	2.6 ng		75103	6	20.18	585588	20.0
Heneicosane	20.62	4.7 ng		137678	6	20.18	585588	20.0
unknown20.91	20.91	3.0 ng		87577	6	20.18	585588	20.0