

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062117\
 Data File : BF096090.D
 Acq On : 21 Jun 2017 18:15
 Operator : SJ/MA
 Sample : I3736-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 G24-1.5-3

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-BF060517.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	1.557	9	12	47	rVB	543235	1236797	83.09%	8.726%
2	4.475	504	508	531	rBV	70029	198985	13.37%	1.404%
3	5.192	626	630	659	rBV	423296	1145684	76.97%	8.083%
4	5.434	667	671	676	rVB3	9527	15005	1.01%	0.106%
5	5.592	693	698	707	rVB	8177	15113	1.02%	0.107%
6	6.869	911	915	925	rBV	455720	990965	66.57%	6.991%
7	6.951	925	929	938	rVV	784534	1488495	100.00%	10.502%
8	7.016	938	940	946	rVV	40054	67662	4.55%	0.477%
9	7.098	950	954	961	rVB	37795	53943	3.62%	0.381%
10	7.286	982	986	997	rBV	294512	402132	27.02%	2.837%
11	7.380	997	1002	1008	rVB2	15981	24869	1.67%	0.175%
12	7.522	1021	1026	1036	rBV	700711	978215	65.72%	6.901%
13	7.839	1075	1080	1089	rVB4	10566	27691	1.86%	0.195%
14	8.210	1139	1143	1161	rBV	407069	707967	47.56%	4.995%
15	8.333	1161	1164	1176	rVB4	31431	55722	3.74%	0.393%
16	9.322	1328	1332	1345	rBV	389442	577861	38.82%	4.077%
17	9.422	1345	1349	1355	rVB3	20397	29515	1.98%	0.208%
18	10.133	1465	1470	1474	rBV3	10752	15125	1.02%	0.107%
19	10.410	1511	1517	1523	rVB2	17748	23602	1.59%	0.167%
20	10.492	1525	1531	1541	rBV	34508	60593	4.07%	0.427%
21	10.645	1551	1557	1563	rBV2	19059	29581	1.99%	0.209%
22	11.098	1629	1634	1645	rBV	1113395	1389422	93.34%	9.803%
23	11.327	1669	1673	1677	rVB	16455	18263	1.23%	0.129%
24	11.510	1700	1704	1706	rBV4	14670	20812	1.40%	0.147%
25	11.627	1720	1724	1728	rBV2	21172	32477	2.18%	0.229%
26	11.668	1728	1731	1740	rVB3	21697	32772	2.20%	0.231%
27	11.798	1749	1753	1765	rBV	81791	135990	9.14%	0.959%
28	11.927	1770	1775	1781	rVB2	11042	19464	1.31%	0.137%
29	12.139	1806	1811	1817	rBV2	446490	588017	39.50%	4.149%
30	12.998	1950	1957	1960	rBV2	25645	34108	2.29%	0.241%
31	13.045	1960	1965	1968	rVB5	8533	14941	1.00%	0.105%
32	13.439	2028	2032	2048	rBV	423949	691927	46.49%	4.882%
33	13.768	2081	2088	2090	rBV2	26118	39487	2.65%	0.279%
34	14.286	2170	2176	2181	rBV9	8834	20064	1.35%	0.142%

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G24-1.5-3

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-BF060517.M
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35	14.498	2209	2212	2214	rBV3	15945	18126	1.22%	0.128%
36	14.533	2214	2218	2223	rVV	378742	515293	34.62%	3.635%
37	14.574	2223	2225	2232	rVB	44265	60337	4.05%	0.426%
38	14.680	2239	2243	2248	rVB2	11566	17389	1.17%	0.123%
39	15.351	2354	2357	2360	rBV	16056	19770	1.33%	0.139%
40	15.398	2362	2365	2370	rVB	23077	27251	1.83%	0.192%
41	15.568	2390	2394	2402	rVB3	76862	99184	6.66%	0.700%
42	16.368	2527	2530	2533	rBV	63891	64685	4.35%	0.456%
43	16.674	2578	2582	2588	rBV	147486	186139	12.51%	1.313%
44	16.921	2619	2624	2631	rBV	776913	953003	64.02%	6.724%
45	18.268	2848	2853	2857	rBV	392714	520630	34.98%	3.673%
46	19.309	3027	3030	3035	rBV	114821	120355	8.09%	0.849%
47	19.944	3135	3138	3149	rVB	282644	388589	26.11%	2.742%

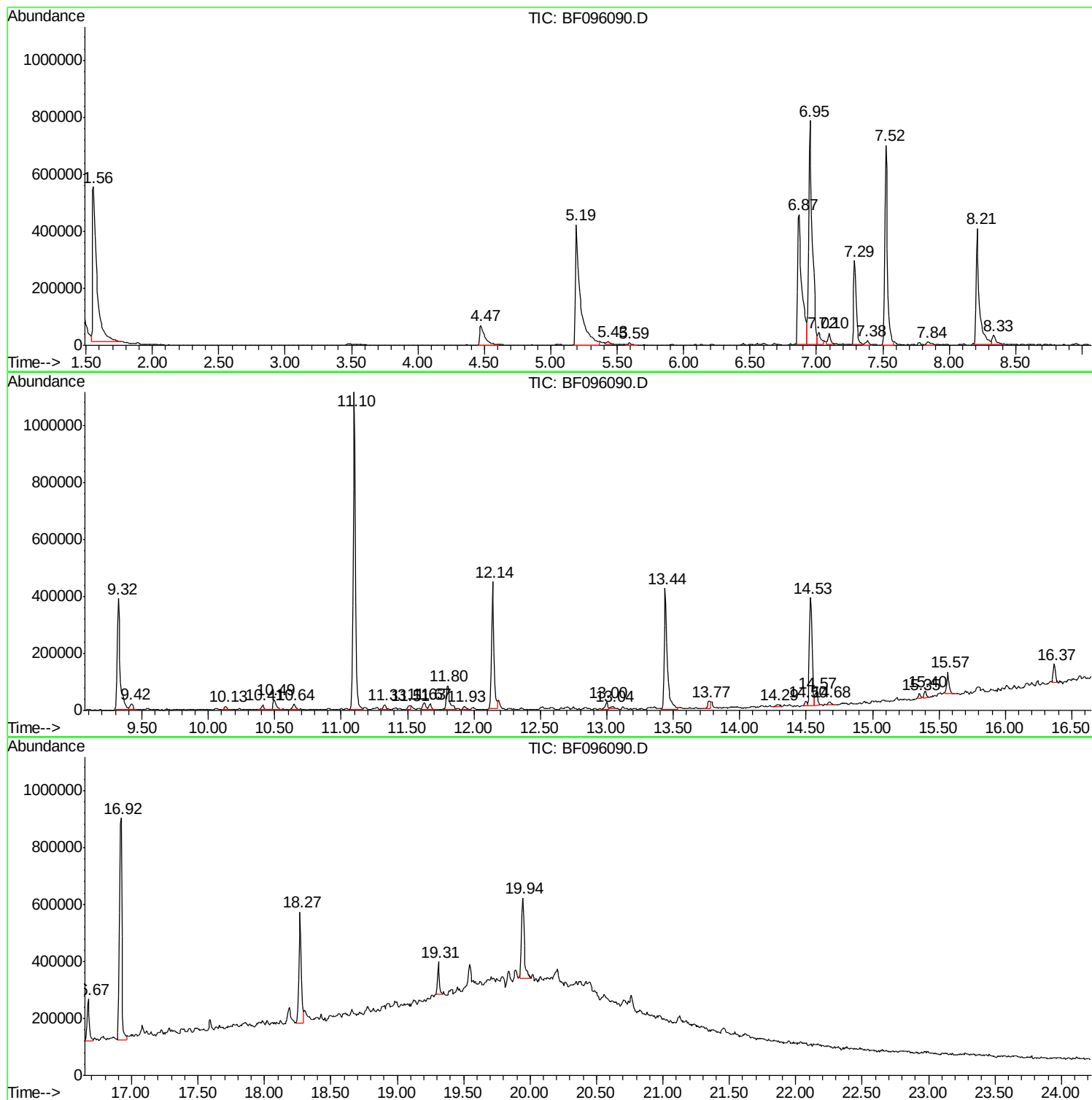
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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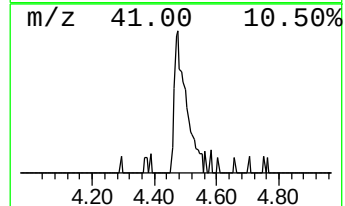
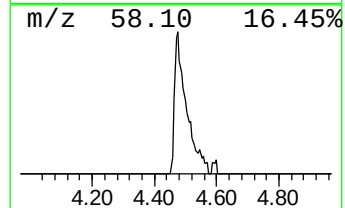
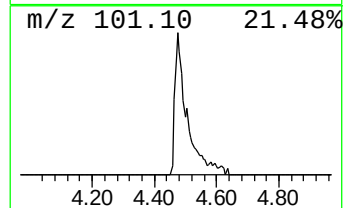
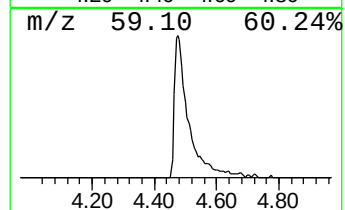
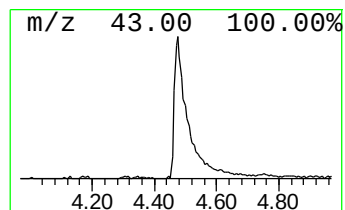
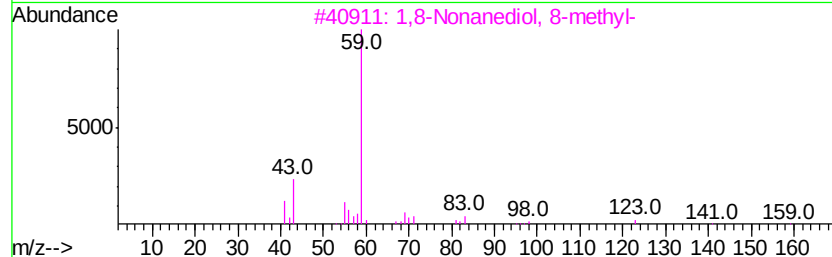
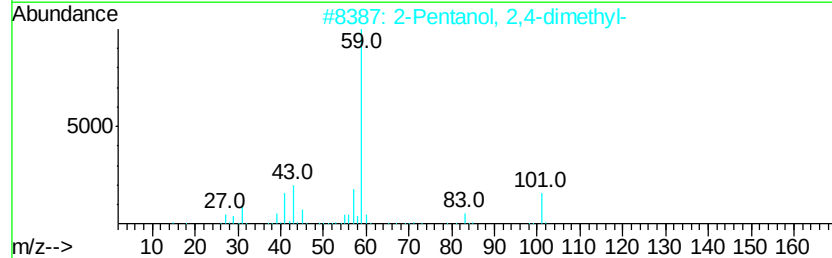
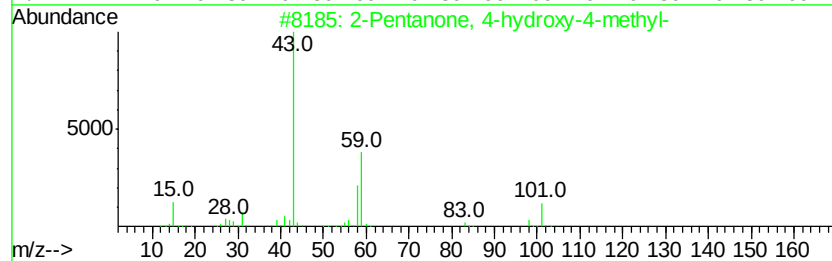
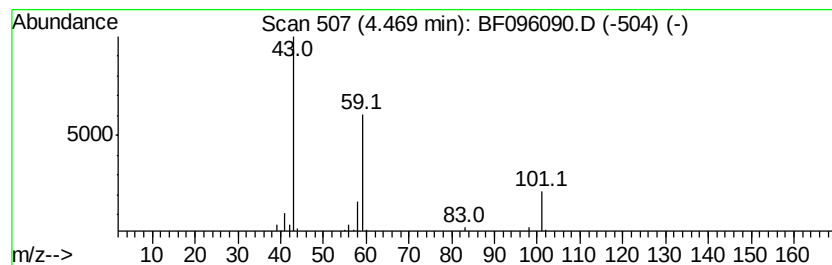
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.47	9.90 ng	198985	1,4-Dichlorobenzene-d4	7.29

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	25
3		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
4		1,2-Butanediol	90	C4H10O2	000584-03-2	25
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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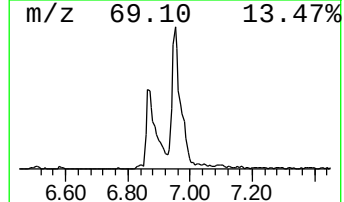
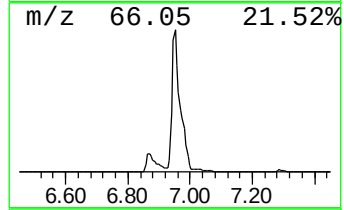
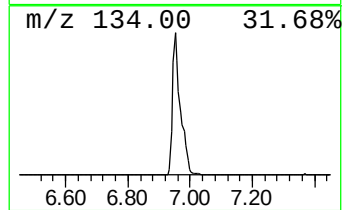
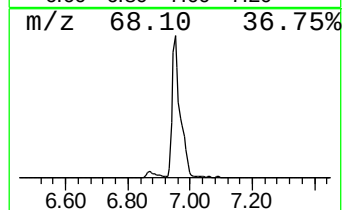
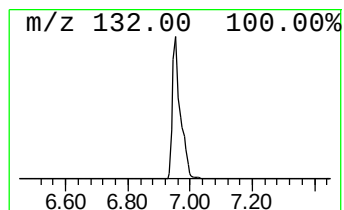
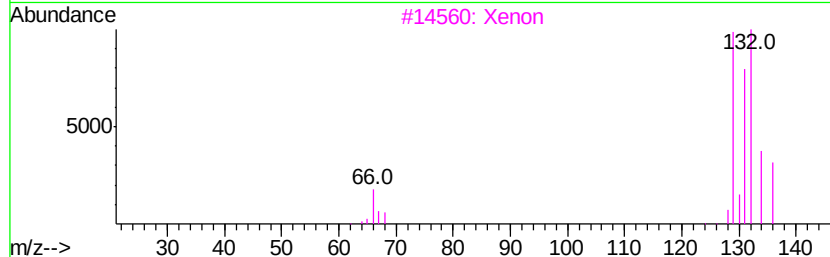
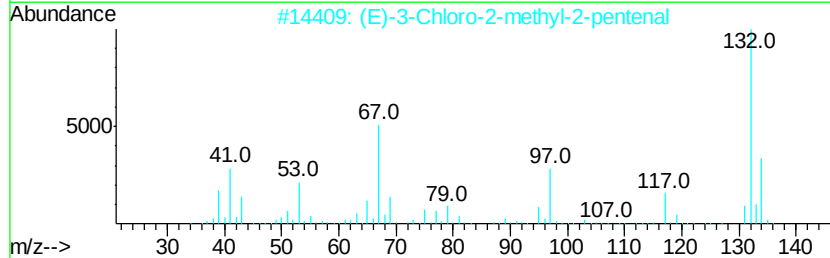
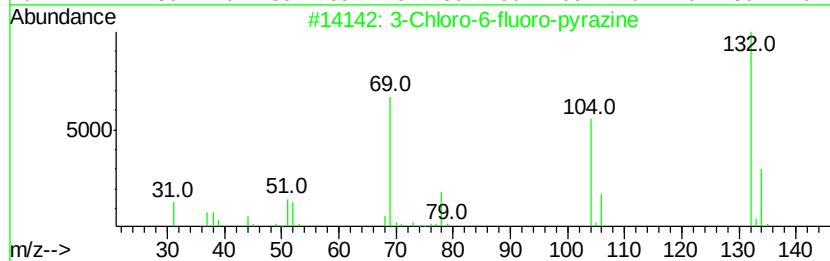
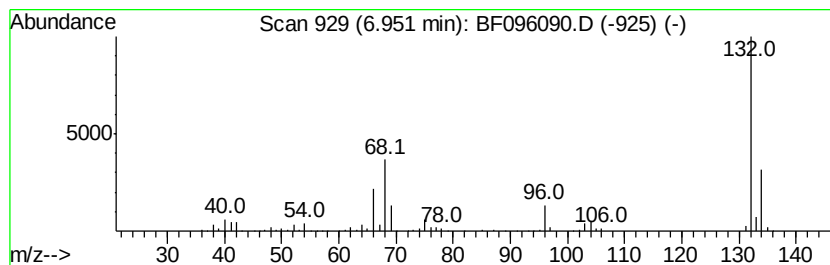
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown6.95 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.95	74.03 ng	1488500	1,4-Dichlorobenzene-d4	7.29

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	12
3		Xenon	132	Xe	007440-63-3	9
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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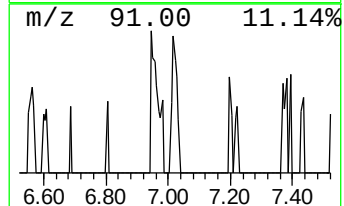
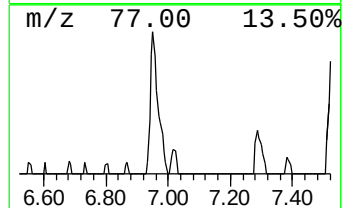
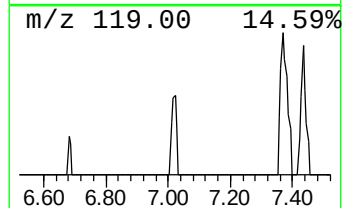
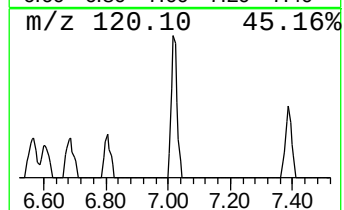
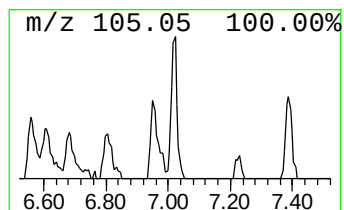
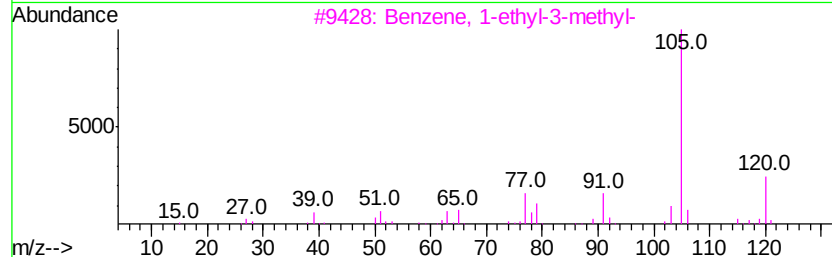
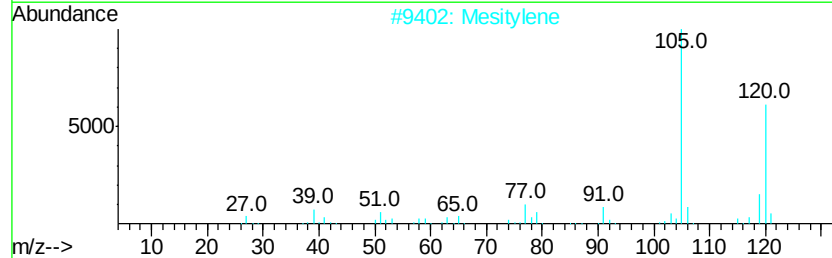
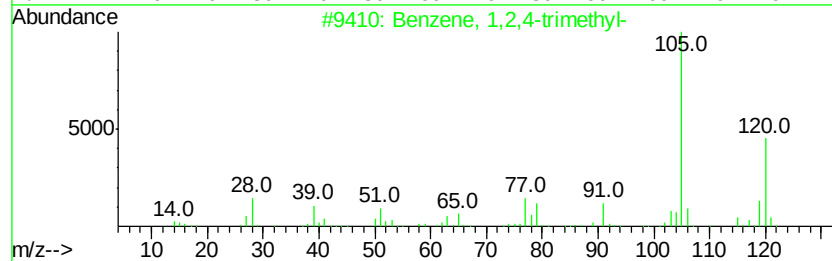
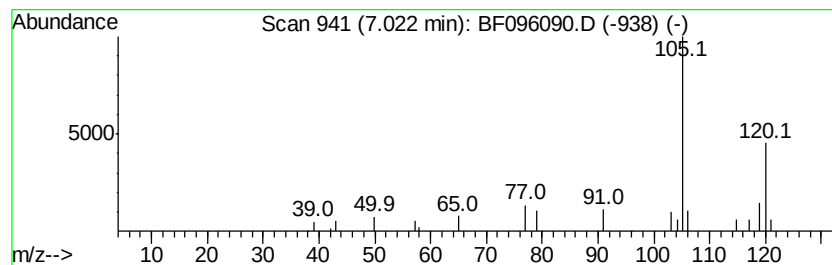
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1,2,4-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.02	3.37 ng	67662	1,4-Dichlorobenzene-d4	7.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
2		Mesitylene	120	C9H12	000108-67-8	91
3		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	87
5		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	87



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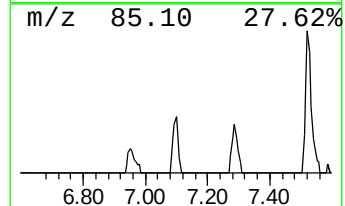
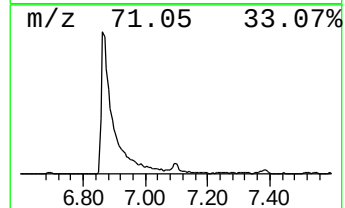
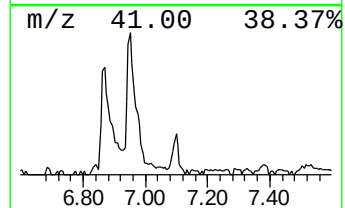
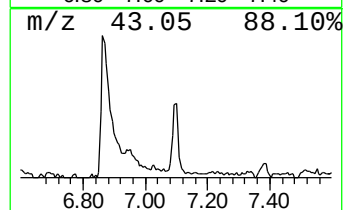
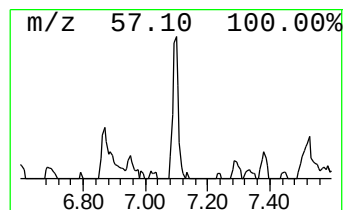
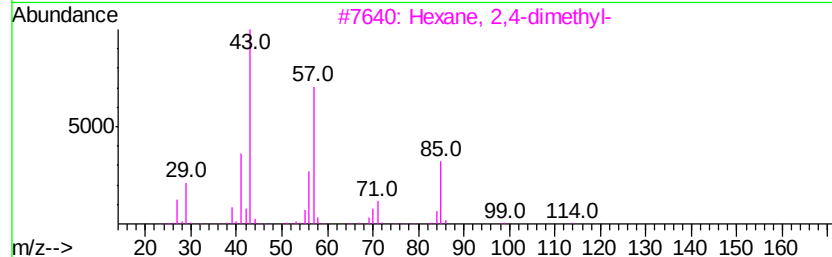
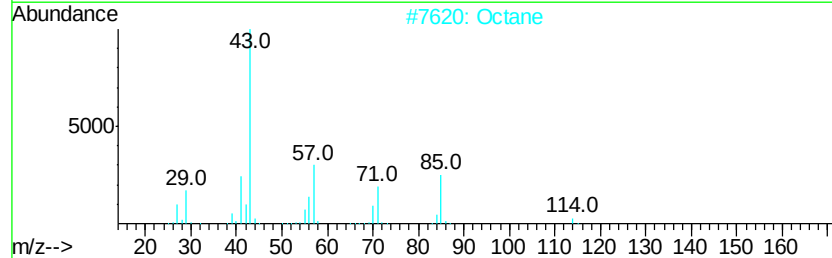
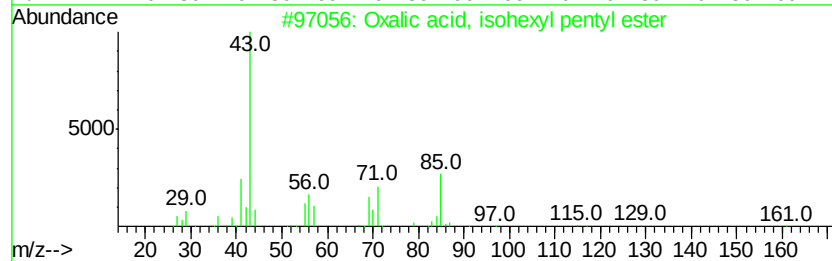
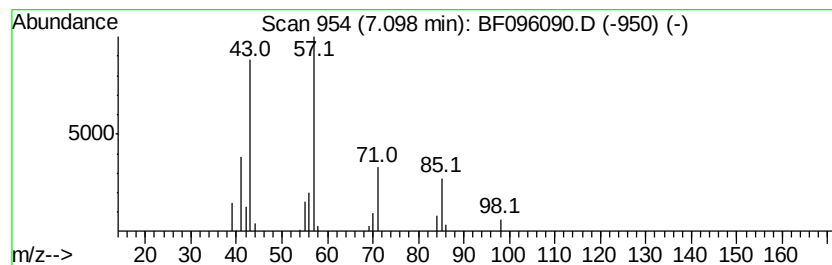
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Oxalic acid, isohexyl penty... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.10	2.68 ng	53943	1,4-Dichlorobenzene-d4	7.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxalic acid, isohexyl pentyl ester	244	C13H24O4	1000309-32-8	64
2		Octane	114	C8H18	000111-65-9	64
3		Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	59
4		Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1000309-37-4	59
5		Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	50



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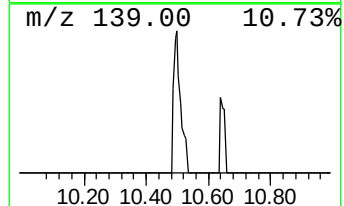
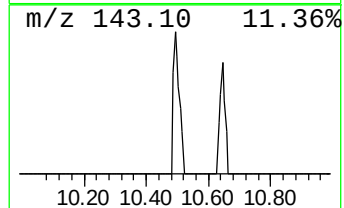
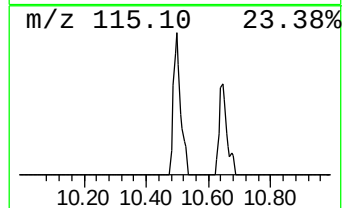
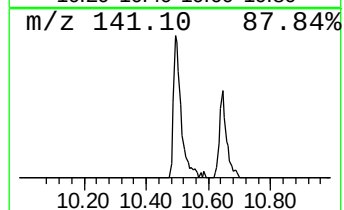
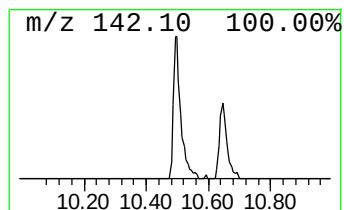
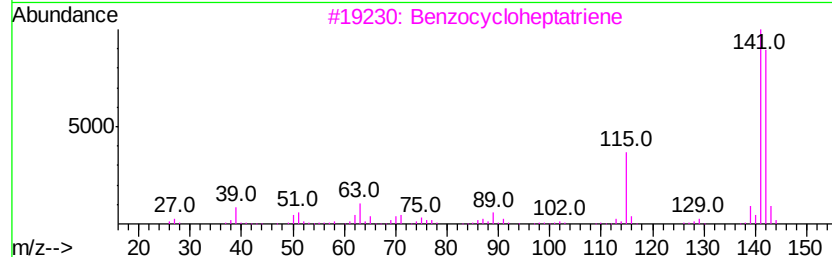
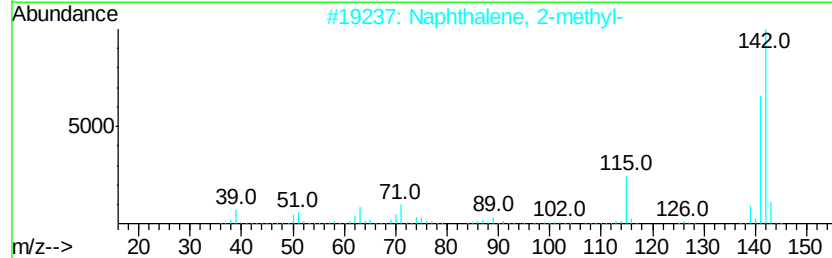
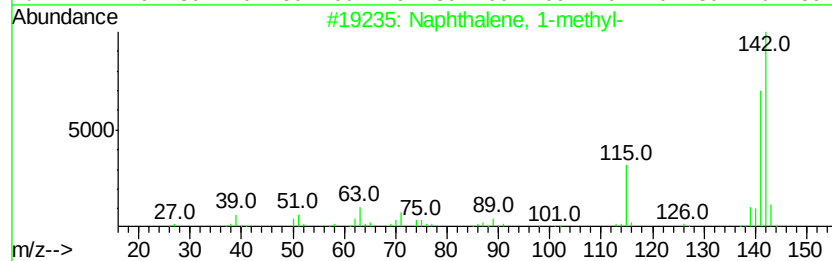
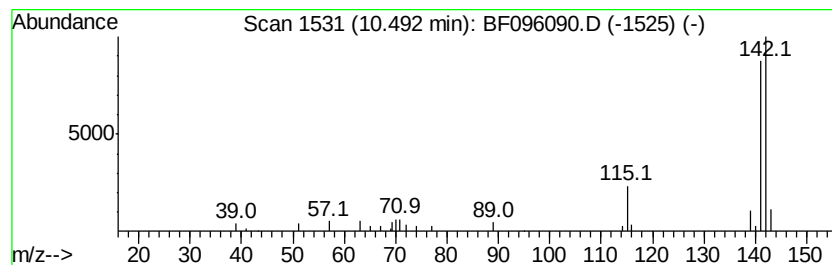
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.49	2.10 ng	60593	Naphthalene-d8	9.32		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
2		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	90
3		Benzocycloheptatriene	142	C11H10	000264-09-5	83
4		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	56
5		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062117\
Data File : BF096090.D
Acq On : 21 Jun 2017 18:15
Operator : SJ/MA
Sample : I3736-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

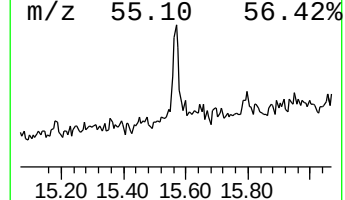
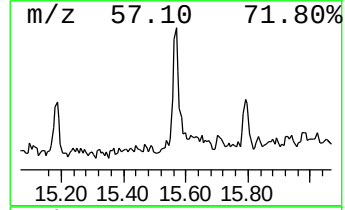
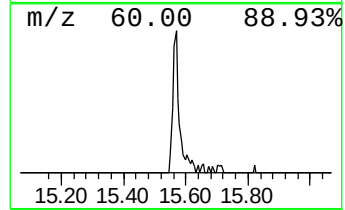
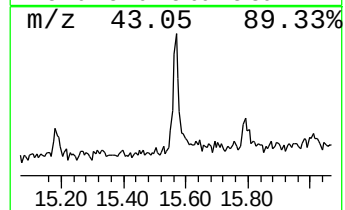
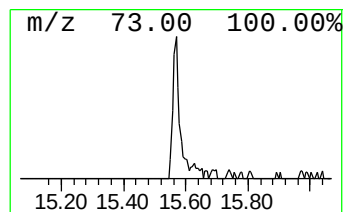
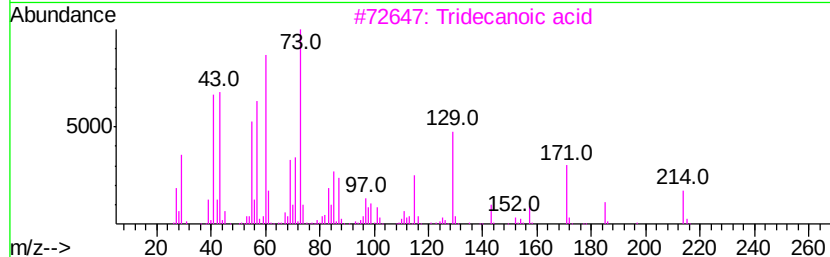
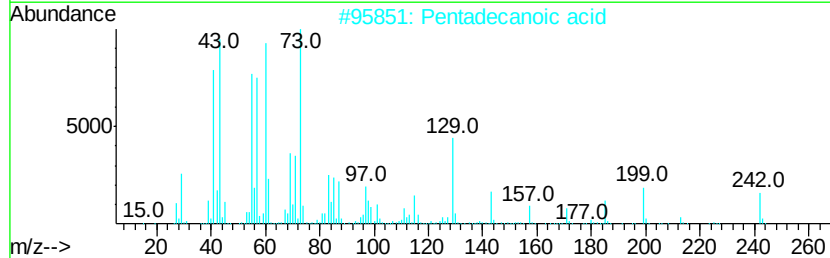
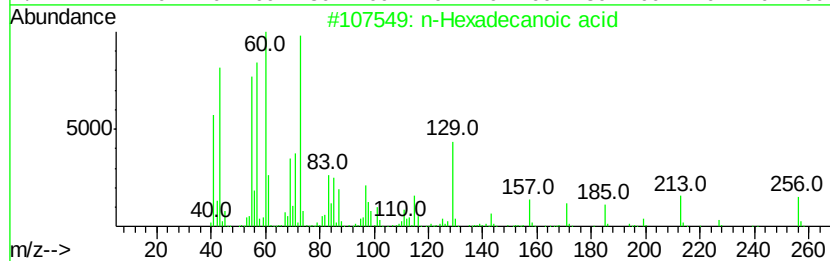
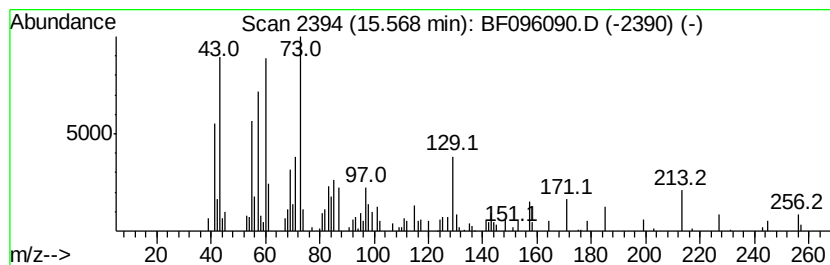
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.57	3.85 ng	99184	Phenanthrene-d10		14.53
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062117\
Data File : BF096090.D
Acq On : 21 Jun 2017 18:15
Operator : SJ/MA
Sample : I3736-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G24-1.5-3

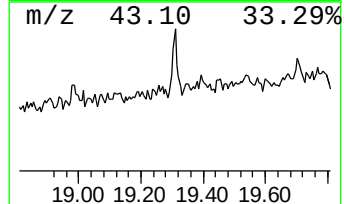
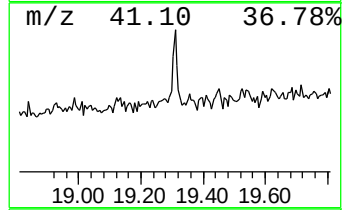
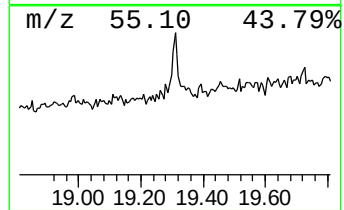
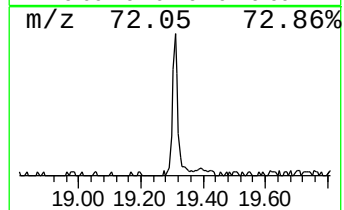
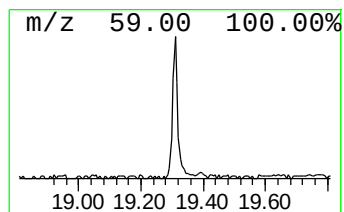
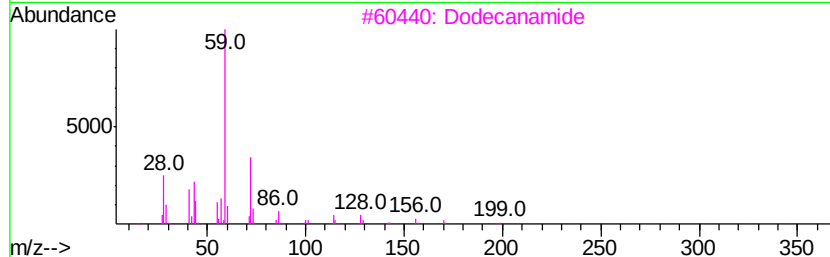
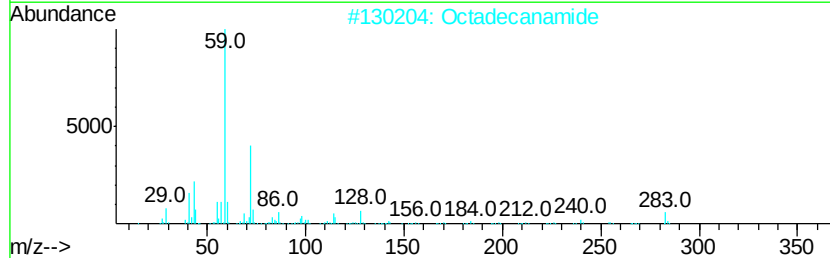
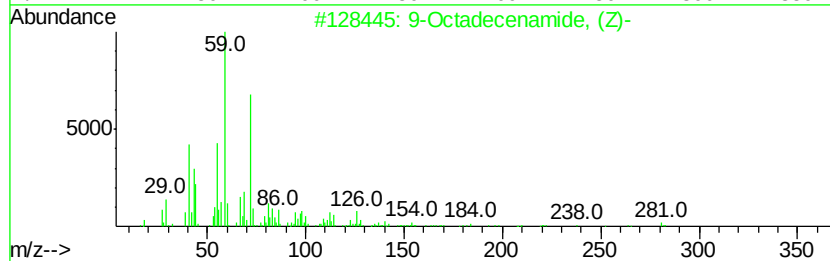
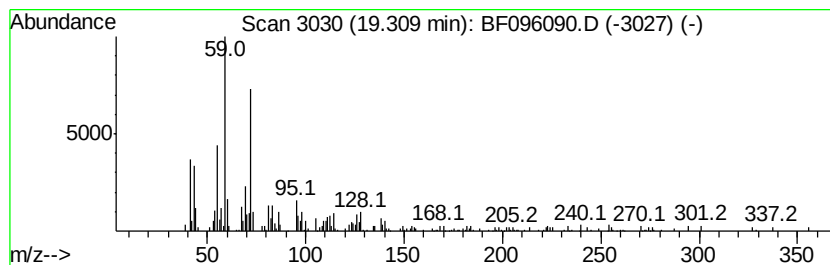
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.31	6.19 ng	120355	Perylene-d12	19.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2		Octadecanamide	283	C18H37NO	000124-26-5	64
3		Dodecanamide	199	C12H25NO	001120-16-7	59
4		Tetradecanamide	227	C14H29NO	000638-58-4	59
5		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	53



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Sample : I3736-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G24-1.5-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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...	4.47	9.9	ng	198985	1	7.29	402132	20.0
unknown6.95	6.95	74.0	ng	1488500	1	7.29	402132	20.0
Benzene, 1,2,4-tr...	7.02	3.4	ng	67662	1	7.29	402132	20.0
Oxalic acid, isoh...	7.10	2.7	ng	53943	1	7.29	402132	20.0
Naphthalene, 1-me...	10.49	2.1	ng	60593	2	9.32	577861	20.0
n-Hexadecanoic acid	15.57	3.9	ng	99184	4	14.53	515293	20.0
9-Octadecenamide,...	19.31	6.2	ng	120355	6	19.94	388589	20.0