

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041318\
 Data File : BF104486.D
 Acq On : 13 Apr 2018 18:41
 Operator : JU/SJ
 Sample : J2152-01 2X
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BU-01-041218

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-BF040618.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	5.010	493	497	504	rVB	87959	96810	5.19%	0.414%
2	5.416	561	566	569	rBV	1772848	1586274	85.06%	6.789%
3	6.051	669	674	681	rBV	23954	33216	1.78%	0.142%
4	6.439	735	740	750	rBV	1660786	1643967	88.15%	7.036%
5	6.575	759	763	766	rBV	1959156	1692443	90.75%	7.244%
6	6.810	799	803	806	rBV	979773	794136	42.58%	3.399%
7	6.963	825	829	832	rBV	1586676	1343406	72.04%	5.750%
8	7.369	894	898	901	rBV	1067455	1000397	53.64%	4.282%
9	8.092	1017	1021	1024	rBV	1329590	1026331	55.03%	4.393%
10	8.680	1117	1121	1125	rBV	25726	22492	1.21%	0.096%
11	9.169	1199	1204	1207	rBV	2301736	1864893	100.00%	7.982%
12	9.245	1213	1217	1219	rBV	48407	38463	2.06%	0.165%
13	9.563	1267	1271	1274	rBV	270861	235754	12.64%	1.009%
14	9.775	1304	1307	1310	rVB	92724	65552	3.52%	0.281%
15	9.851	1316	1320	1323	rBV	1221407	1078800	57.85%	4.617%
16	9.880	1323	1325	1329	rVB	88856	68645	3.68%	0.294%
17	10.051	1349	1354	1358	rVB	44139	46996	2.52%	0.201%
18	10.274	1389	1392	1395	rVB	101218	75262	4.04%	0.322%
19	10.398	1410	1413	1418	rVB	75159	69939	3.75%	0.299%
20	10.498	1425	1430	1433	rBV2	24312	35533	1.91%	0.152%
21	10.639	1450	1454	1464	rVB	1079341	974184	52.24%	4.169%
22	10.751	1470	1473	1477	rBV	81657	90742	4.87%	0.388%
23	11.198	1543	1549	1551	rBV2	54849	48708	2.61%	0.208%
24	11.233	1551	1555	1561	rVB3	36593	43488	2.33%	0.186%
25	11.339	1569	1573	1575	rBV	1098253	948163	50.84%	4.058%
26	11.363	1575	1577	1580	rVV	437987	328974	17.64%	1.408%
27	11.410	1583	1585	1589	rVB	109508	92202	4.94%	0.395%
28	11.569	1606	1612	1617	rBV	50320	58475	3.14%	0.250%
29	11.627	1620	1622	1624	rBV2	31196	24460	1.31%	0.105%
30	11.727	1635	1639	1646	rVB	579111	445352	23.88%	1.906%
31	11.839	1655	1658	1660	rBV	32841	26202	1.41%	0.112%
32	11.868	1660	1663	1665	rVB	41630	37582	2.02%	0.161%
33	11.951	1674	1677	1680	rBV	53489	56443	3.03%	0.242%
34	12.033	1685	1691	1696	rBV4	22588	34773	1.86%	0.149%

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ClientSampleId :
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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-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.192	1715	1718	1724	rVB2	44742	38528	2.07%	0.165%
36	12.416	1753	1756	1758	rBV	1302447	1192991	63.97%	5.106%
37	12.439	1758	1760	1767	rVV	1598786	1380180	74.01%	5.907%
38	12.521	1771	1774	1776	rBV	230224	179168	9.61%	0.767%
39	12.551	1776	1779	1783	rVB	378997	317567	17.03%	1.359%
40	12.780	1812	1818	1823	rBV	296737	336578	18.05%	1.441%
41	12.827	1823	1826	1831	rVB3	20674	29573	1.59%	0.127%
42	12.927	1839	1843	1846	rVB	1506269	1325891	71.10%	5.675%
43	12.998	1851	1855	1859	rBV3	19137	32203	1.73%	0.138%
44	13.063	1863	1866	1868	rBV	169368	144528	7.75%	0.619%
45	13.110	1871	1874	1879	rVB	59421	60971	3.27%	0.261%
46	13.174	1882	1885	1888	rVB2	65913	59593	3.20%	0.255%
47	13.215	1888	1892	1894	rBV2	23549	25590	1.37%	0.110%
48	13.815	1992	1994	1999	rVB2	148170	158417	8.49%	0.678%
49	13.980	2016	2022	2025	rBV2	873790	944439	50.64%	4.042%
50	14.004	2025	2026	2032	rVB	133025	123109	6.60%	0.527%
51	14.086	2038	2040	2043	rVB	30194	23324	1.25%	0.100%
52	14.462	2101	2104	2107	rBV3	43368	45475	2.44%	0.195%
53	15.021	2196	2199	2202	rBV	104093	148842	7.98%	0.637%
54	15.092	2209	2211	2214	rBV2	41898	49199	2.64%	0.211%
55	15.386	2258	2261	2267	rVB	72061	82797	4.44%	0.354%
56	15.451	2267	2272	2282	rVB	474563	636624	34.14%	2.725%

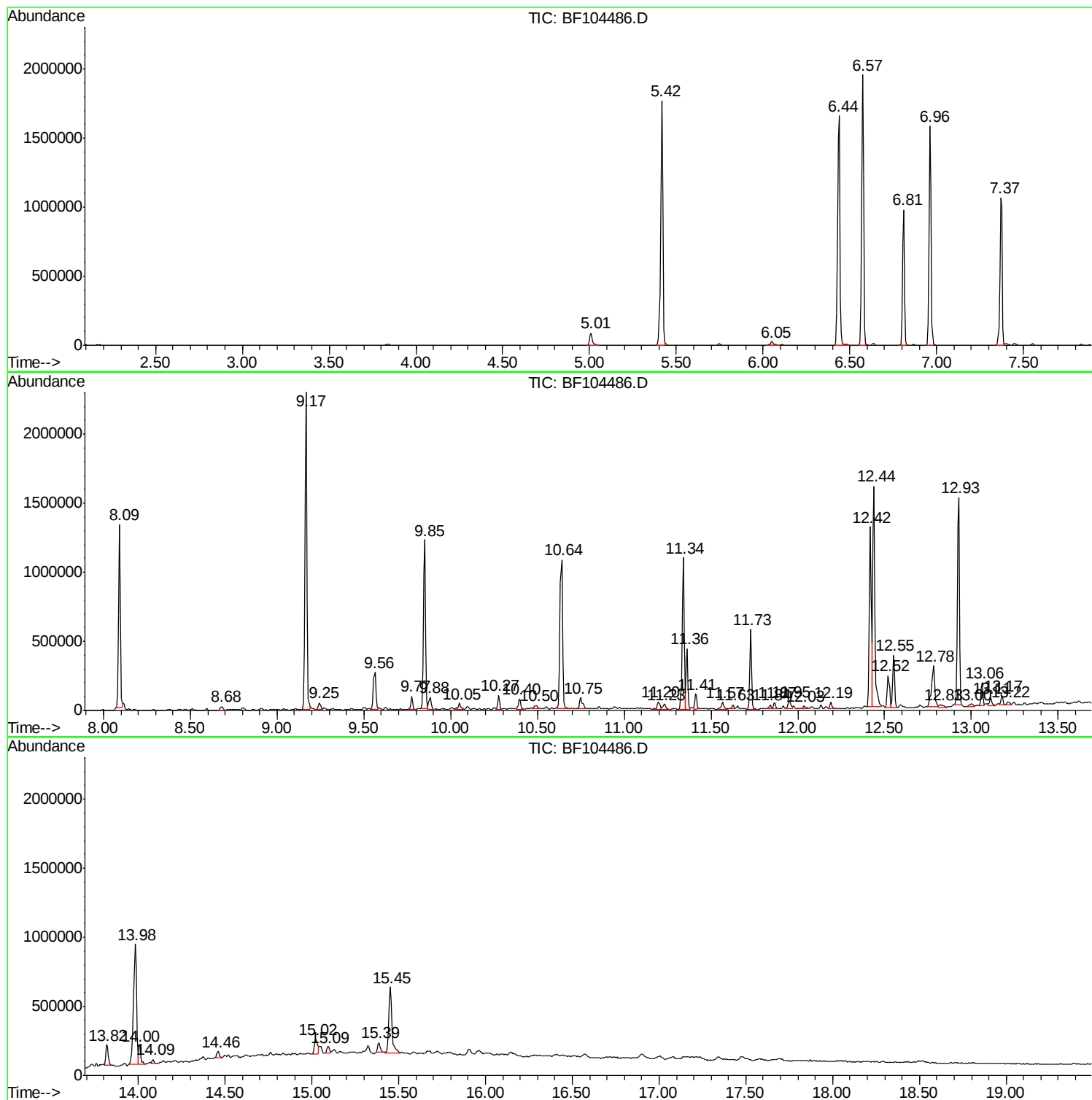
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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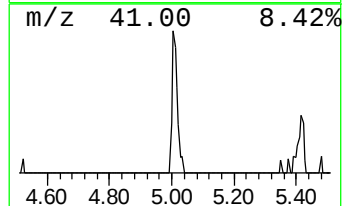
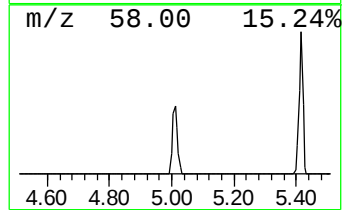
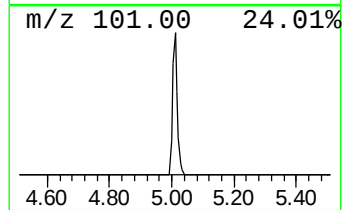
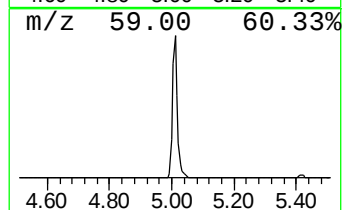
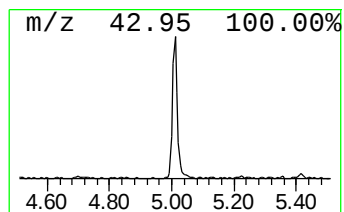
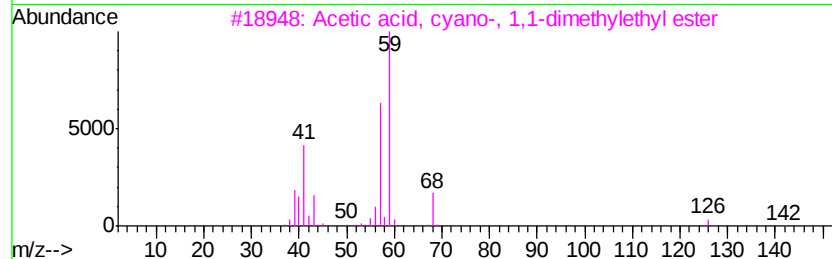
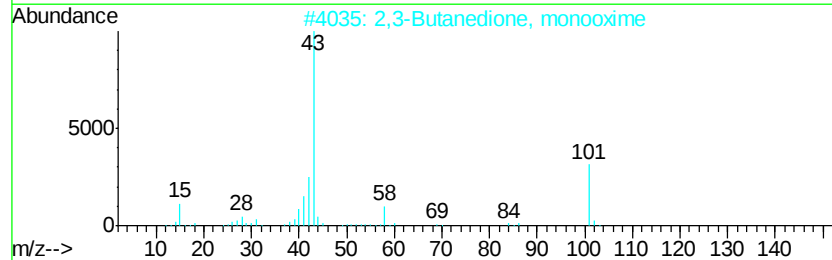
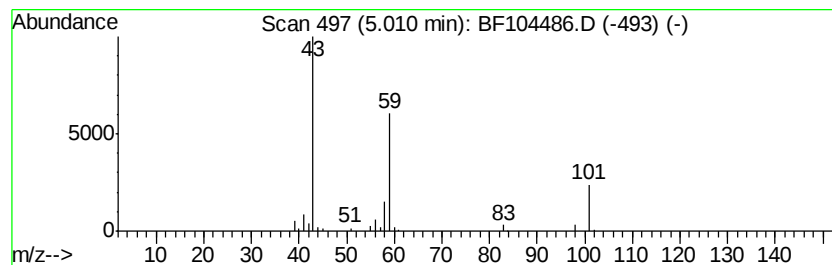
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	2.44 ng	96810	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		5-Hexen-2-one	98	C6H10O	000109-49-9	10
5		1,2-Butanediol	90	C4H10O2	000584-03-2	9



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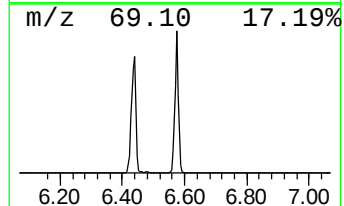
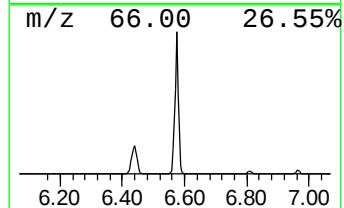
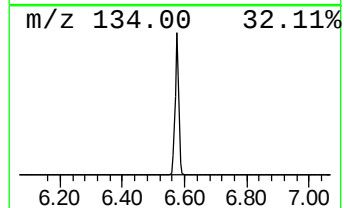
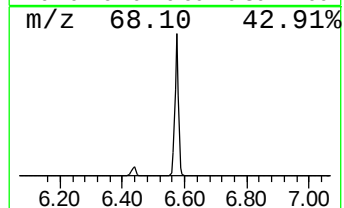
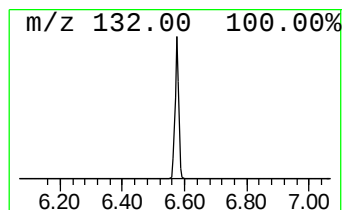
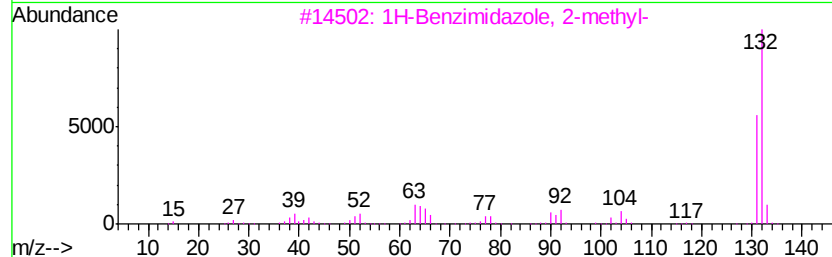
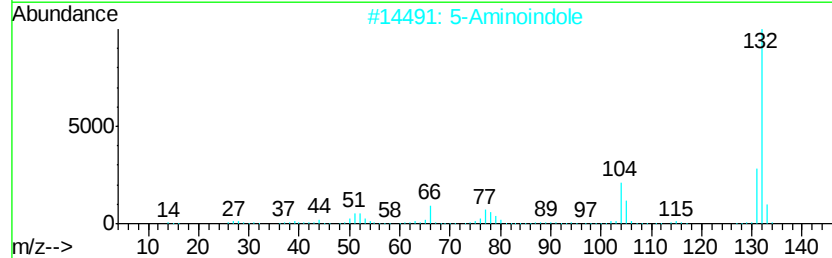
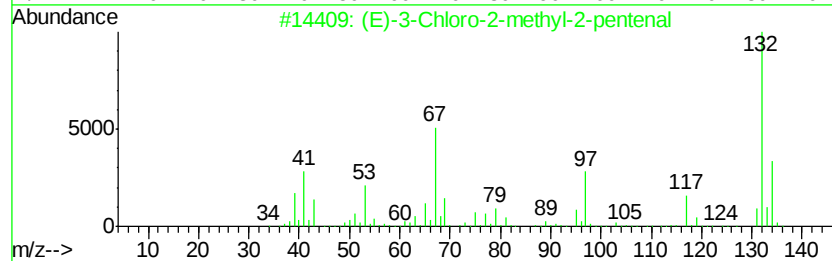
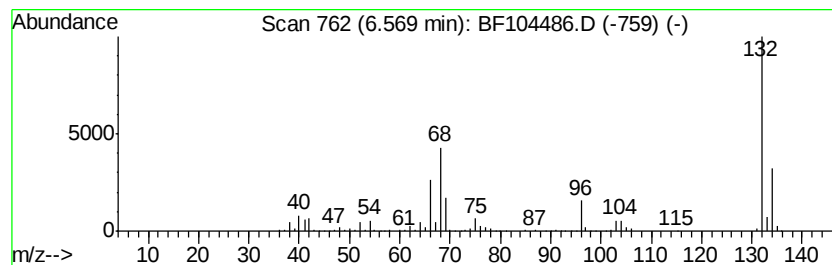
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	42.62 ng	1692440	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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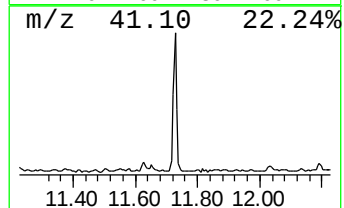
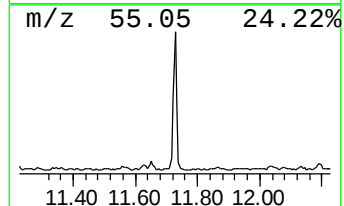
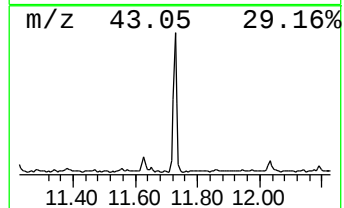
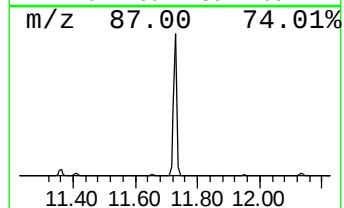
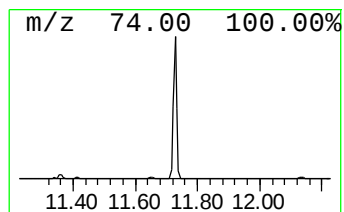
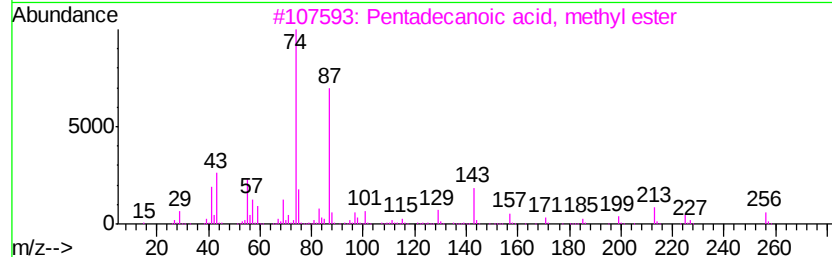
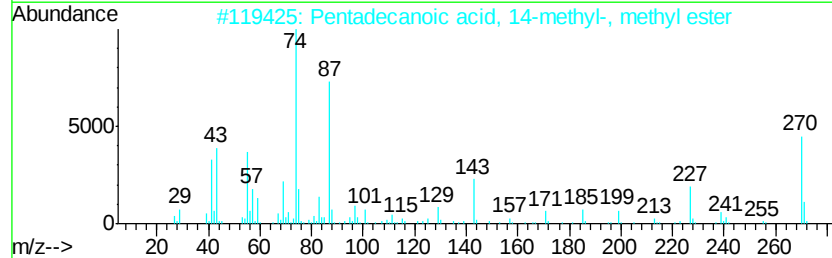
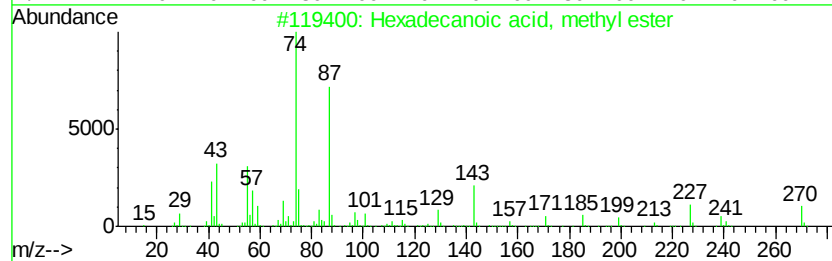
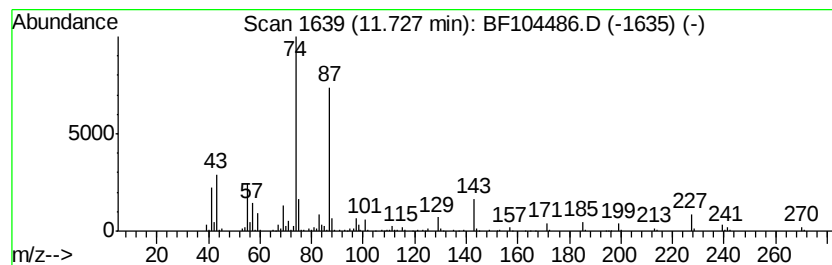
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.73	9.39 ng	445352	Phenanthrene-d10	11.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	90
3		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4		Methyl tetradecanoate	242	C15H30O2	000124-10-7	86
5		Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	86



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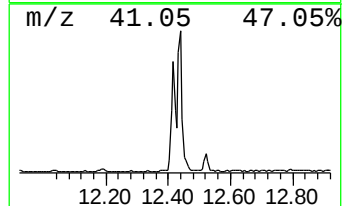
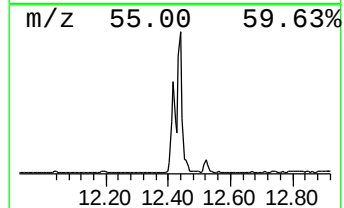
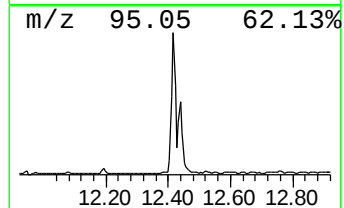
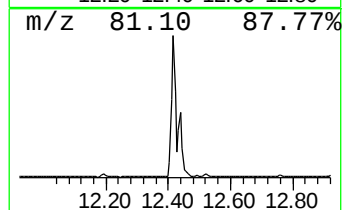
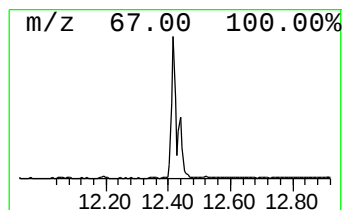
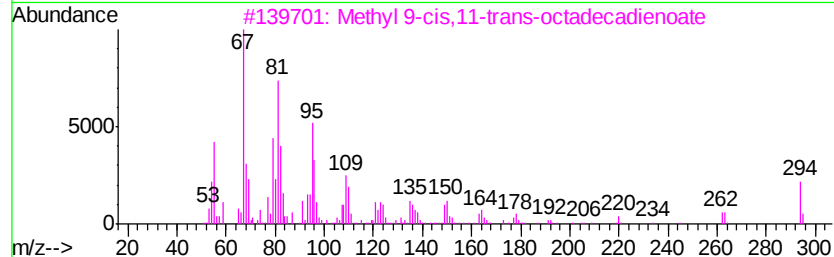
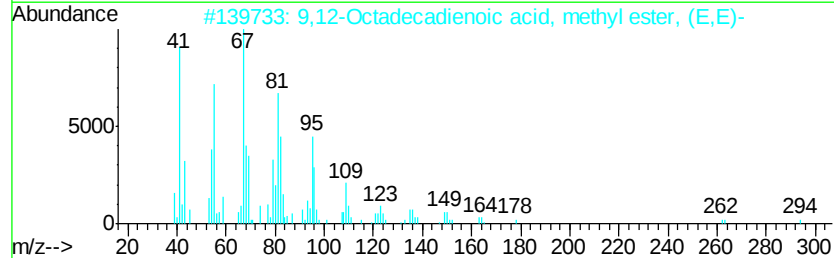
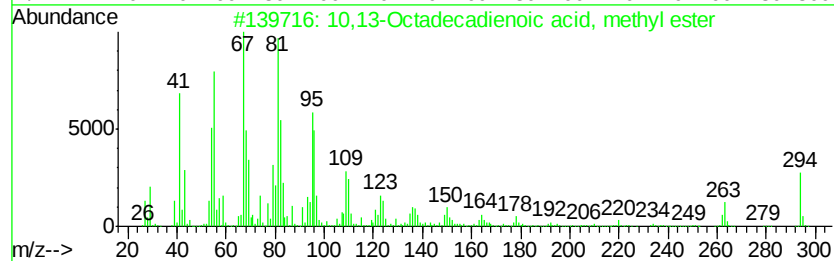
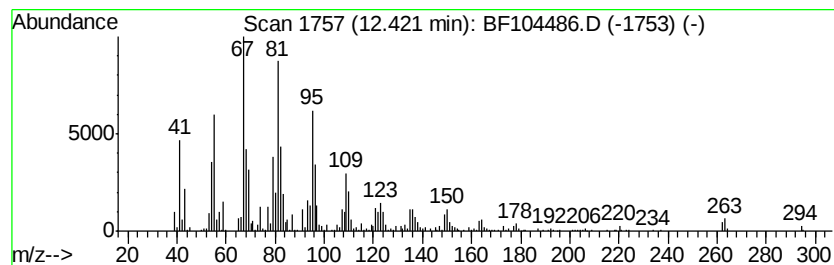
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 10,13-Octadecadienoic acid,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.42	25.16 ng	1192990	Phenanthrene-d10	11.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
2		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
3		Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99
4		8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99
5		9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99



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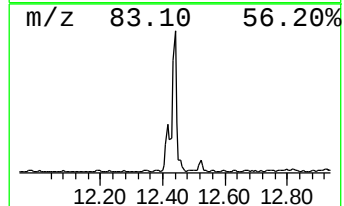
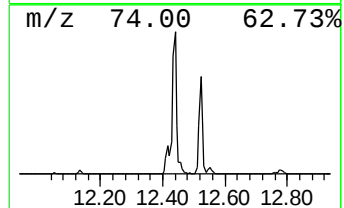
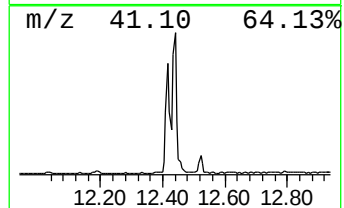
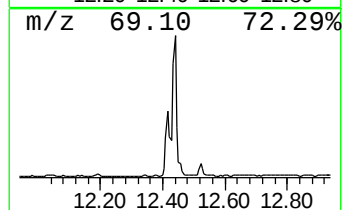
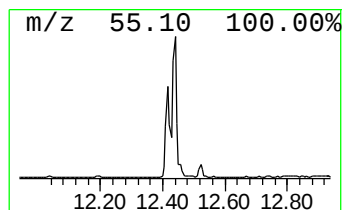
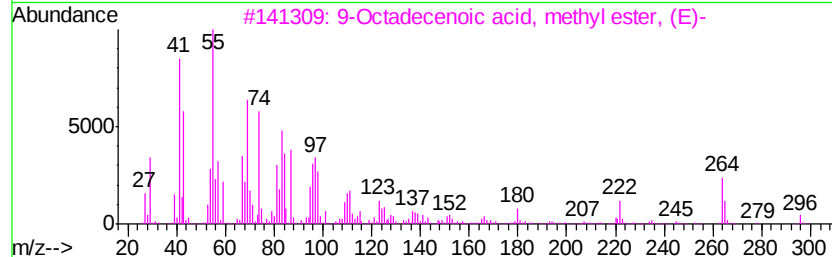
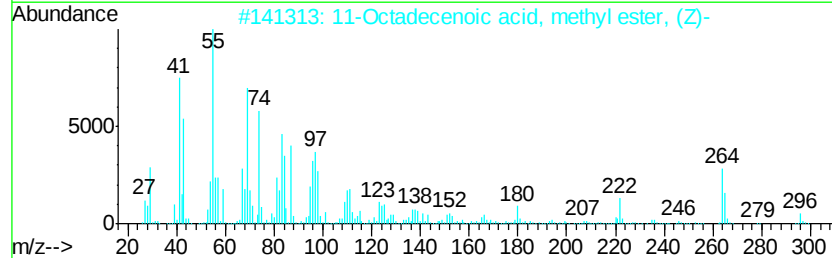
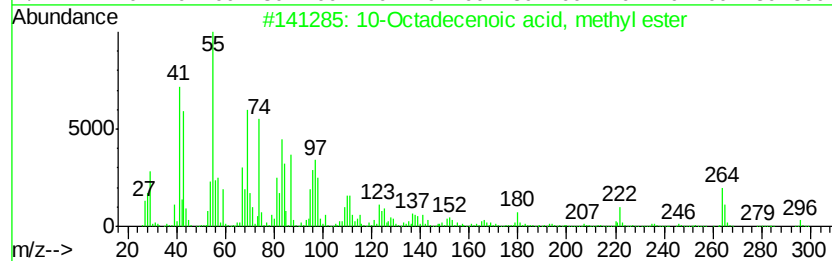
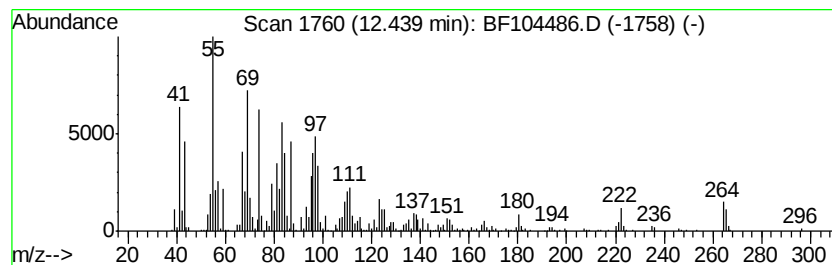
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 10-Octadecenoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.44	29.11 ng	1380180	Phenanthrene-d10	11.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
2		11-Octadecenoic acid, methyl ester	296	C19H36O2	001937-63-9	99
3		9-Octadecenoic acid, methyl ester	296	C19H36O2	001937-62-8	99
4		15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
5		9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041318\
Data File : BF104486.D
Acq On : 13 Apr 2018 18:41
Operator : JU/SJ
Sample : J2152-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-01-041218

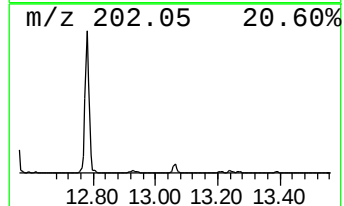
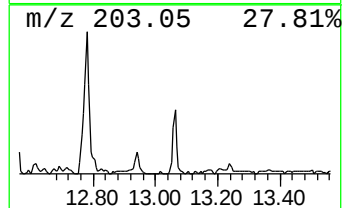
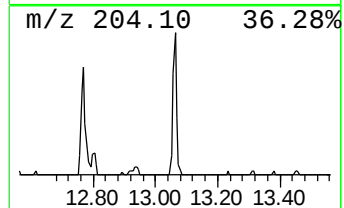
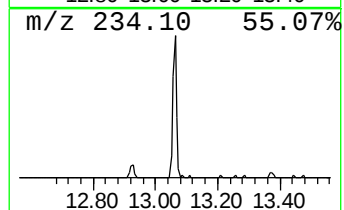
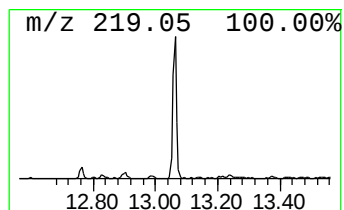
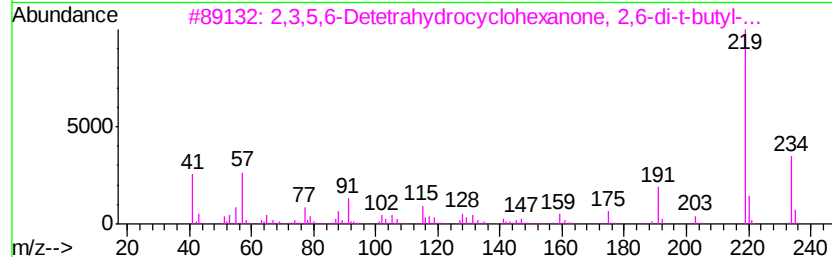
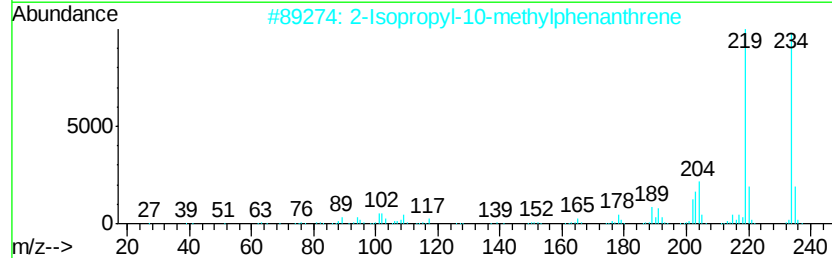
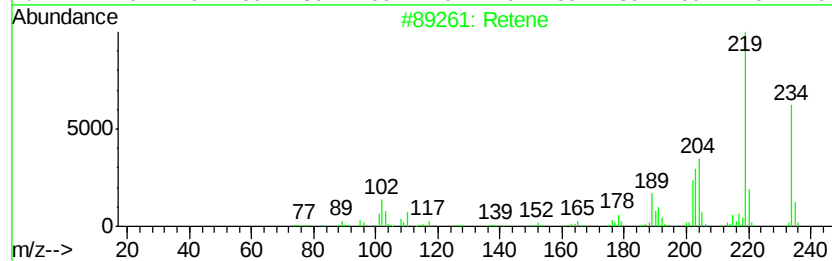
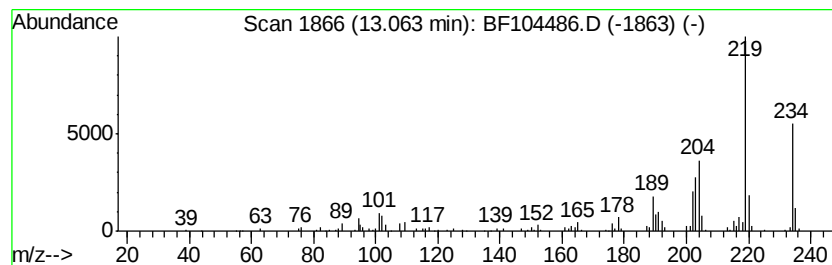
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Retene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.06	3.06 ng	144528	Chrysene-d12	13.98

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Retene	234	C18H18	000483-65-8	98
2			2-Isopropyl-10-methylphenanthrene	234	C18H18	066552-97-4	94
3			2,3,5,6-Tetrahydrocyclohexanon...	234	C15H22O2	101100-38-3	50
4			3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	50
5			Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	49



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041318\
Data File : BF104486.D
Acq On : 13 Apr 2018 18:41
Operator : JU/SJ
Sample : J2152-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-01-041218

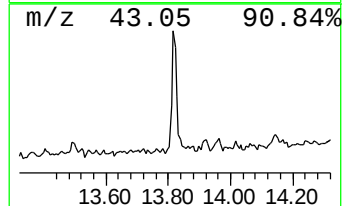
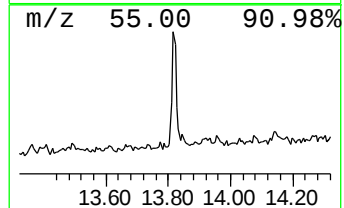
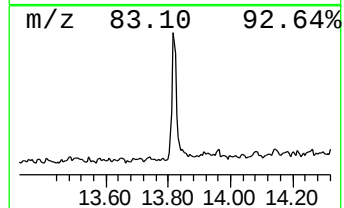
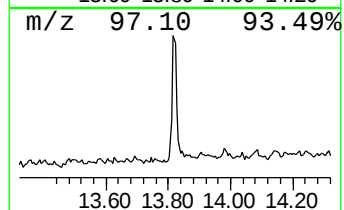
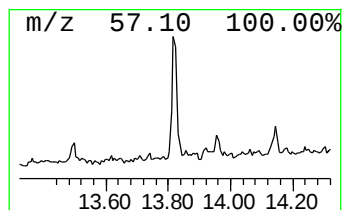
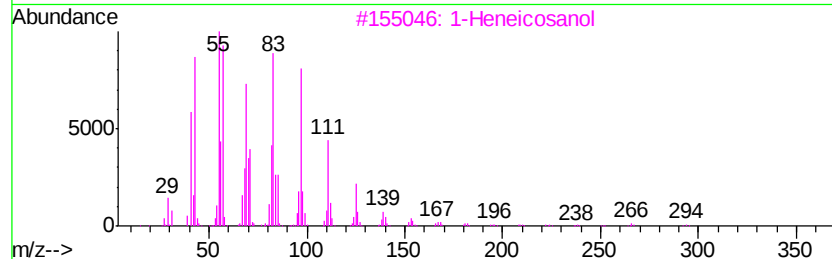
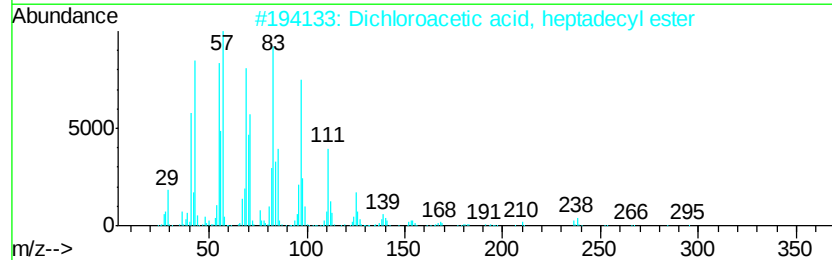
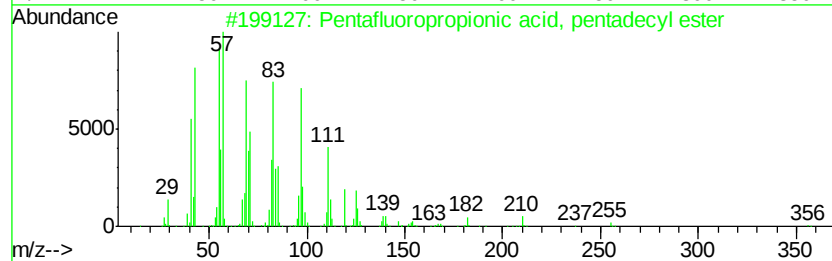
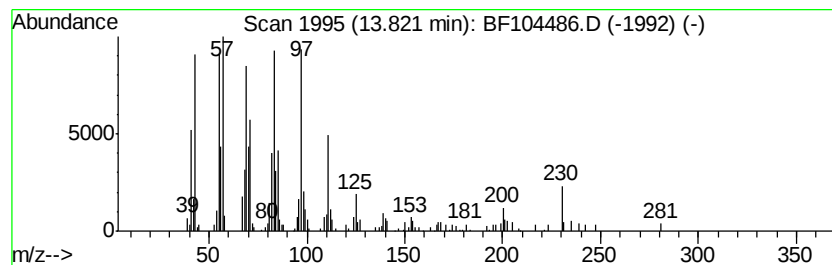
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	3.35 ng	158417	Chrysene-d12	13.98

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
2		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041318\
Data File : BF104486.D
Acq On : 13 Apr 2018 18:41
Operator : JU/SJ
Sample : J2152-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-01-041218

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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...	5.01	2.4	ng	96810	1	6.81	794136	20.0
unknown6.57	6.57	42.6	ng	1692440	1	6.81	794136	20.0
Hexadecanoic acid...	11.73	9.4	ng	445352	4	11.34	948163	20.0
10,13-Octadecadie...	12.42	25.2	ng	1192990	4	11.34	948163	20.0
10-Octadecenoic a...	12.44	29.1	ng	1380180	4	11.34	948163	20.0
Retene	13.06	3.1	ng	144528	5	13.98	944439	20.0
Pentafluoropropio...	13.82	3.4	ng	158417	5	13.98	944439	20.0