

Data Path : Z:\HPCHEM1\BNA F\Data\BF042117\
 Data File : BF094565.D
 Acq On : 21 Apr 2017 16:27
 Operator : SJ/MA
 Sample : I2783-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C-9

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-BF041717.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	2.701	127	130	138	rBV	64584	79539	2.30%	0.296%
2	3.366	236	243	246	rBV	2881085	3458701	100.00%	12.861%
3	3.919	329	337	340	rBV	2054816	3116347	90.10%	11.588%
4	4.313	401	404	415	rBV	243812	238416	6.89%	0.887%
5	5.384	582	586	604	rBV	1533392	1533008	44.32%	5.700%
6	5.507	604	607	612	rVV	763907	683605	19.76%	2.542%
7	5.760	646	650	655	rBV	737410	644237	18.63%	2.396%
8	5.936	676	680	684	rBV	2244670	2095454	60.58%	7.792%
9	6.136	710	714	720	rBV	46121	52447	1.52%	0.195%
10	6.407	755	760	764	rBV	1460918	1587005	45.88%	5.901%
11	7.254	900	904	907	rBV	951727	838133	24.23%	3.117%
12	8.578	1124	1129	1132	rBV	3309010	3174212	91.77%	11.803%
13	9.077	1209	1214	1218	rBV	575684	560234	16.20%	2.083%
14	9.383	1260	1266	1271	rBV2	960728	1038100	30.01%	3.860%
15	9.983	1364	1368	1373	rBV	95847	84501	2.44%	0.314%
16	10.260	1410	1415	1417	rBV2	36017	40197	1.16%	0.149%
17	10.360	1428	1432	1437	rBV5	32185	47218	1.37%	0.176%
18	10.566	1464	1467	1469	rBV	120893	120503	3.48%	0.448%
19	11.119	1558	1561	1565	rBV	95049	93625	2.71%	0.348%
20	11.160	1565	1568	1571	rVV	38697	41441	1.20%	0.154%
21	11.207	1571	1576	1578	rVV	941497	968352	28.00%	3.601%
22	11.230	1578	1580	1585	rVV	236697	226015	6.53%	0.840%
23	11.295	1588	1591	1595	rVB	40167	40764	1.18%	0.152%
24	11.348	1595	1600	1605	rBV	55369	67609	1.95%	0.251%
25	11.560	1633	1636	1639	rBV	42190	51731	1.50%	0.192%
26	11.648	1648	1651	1656	rVB	97241	91350	2.64%	0.340%
27	11.830	1678	1682	1684	rBV	46703	49597	1.43%	0.184%
28	11.860	1684	1687	1694	rVB	51500	65790	1.90%	0.245%
29	11.960	1699	1704	1707	rBV3	46764	56950	1.65%	0.212%
30	12.148	1733	1736	1741	rVB	68392	70860	2.05%	0.263%
31	12.271	1755	1757	1764	rVB3	42832	39432	1.14%	0.147%
32	12.507	1793	1797	1801	rBV2	32148	46799	1.35%	0.174%
33	12.630	1815	1818	1822	rVB	42143	46186	1.34%	0.172%
34	12.695	1825	1829	1832	rBV	232083	247535	7.16%	0.920%

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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-BF041717.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.965	1872	1875	1880	rVB	235010	248651	7.19%	0.925%
36	13.183	1907	1912	1916	rBV	2417011	2838086	82.06%	10.553%
37	13.342	1935	1939	1942	rBV5	32671	53109	1.54%	0.197%
38	13.507	1963	1967	1969	rBV5	38656	47704	1.38%	0.177%
39	13.718	2001	2003	2007	rVB4	34128	39059	1.13%	0.145%
40	14.348	2107	2110	2118	rVB3	69103	125575	3.63%	0.467%
41	14.448	2122	2127	2131	rBV	671782	824442	23.84%	3.066%
42	15.130	2241	2243	2248	rVB5	35697	43223	1.25%	0.161%
43	15.677	2332	2336	2338	rBV	65872	87920	2.54%	0.327%
44	15.848	2362	2365	2370	rBV3	49629	73889	2.14%	0.275%
45	15.959	2382	2384	2390	rVB	44981	61109	1.77%	0.227%
46	16.018	2391	2394	2399	rVV	53234	66724	1.93%	0.248%
47	16.077	2399	2404	2411	rVB	599602	708452	20.48%	2.634%
48	16.571	2485	2488	2493	rVB4	53451	78875	2.28%	0.293%

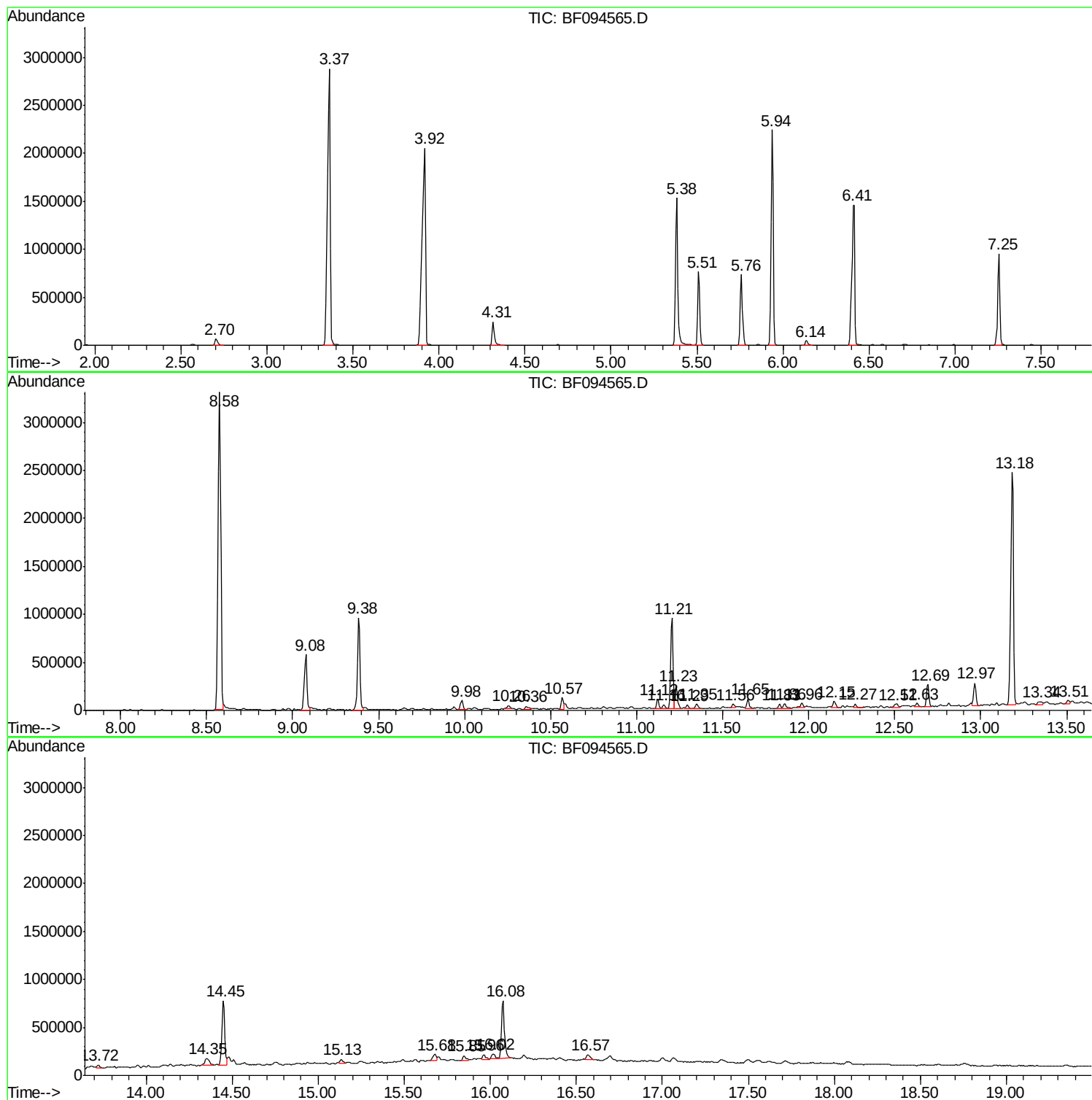
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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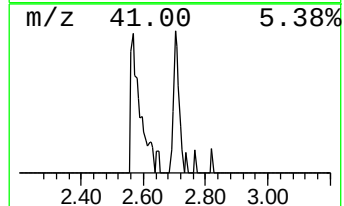
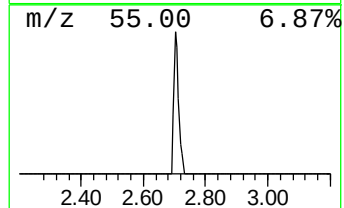
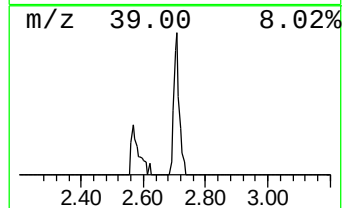
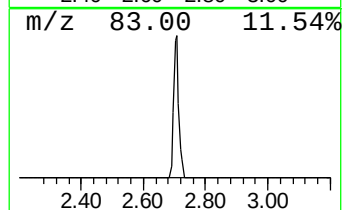
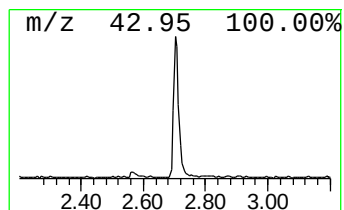
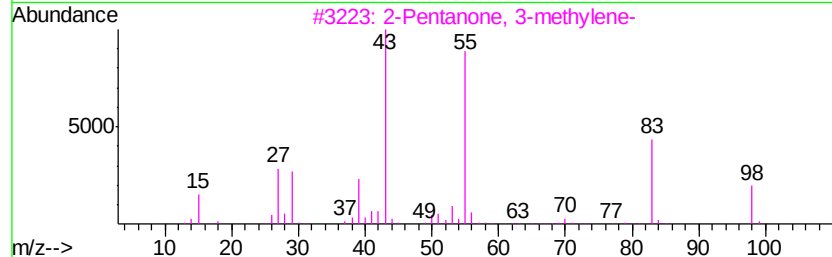
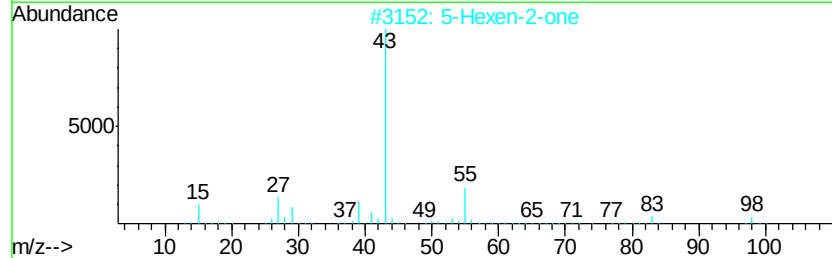
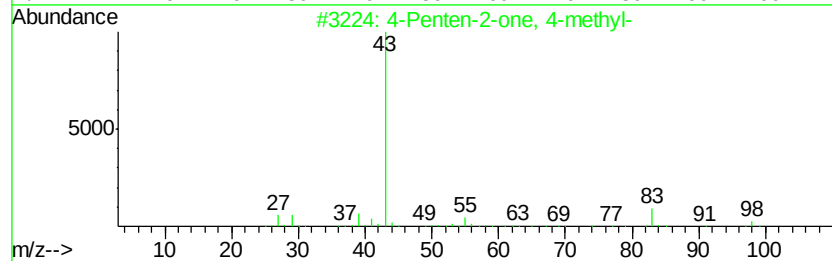
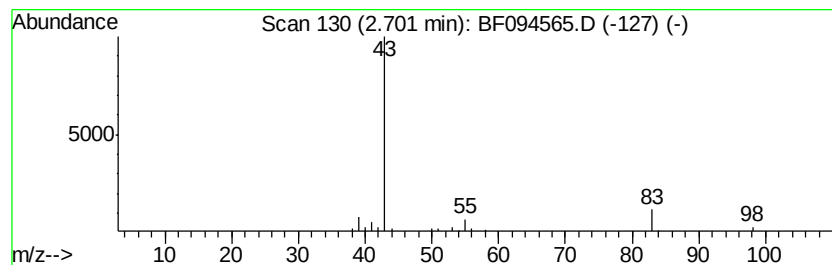
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.70	2.47 ng	79539	1,4-Dichlorobenzene-d4	5.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2		5-Hexen-2-one	98	C6H10O	000109-49-9	50
3		2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	23
4		Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	9
5		4-Hexen-2-one	98	C6H10O	025659-22-7	9



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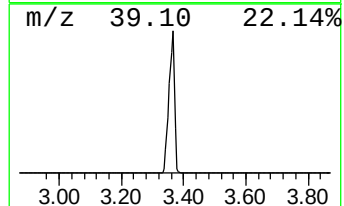
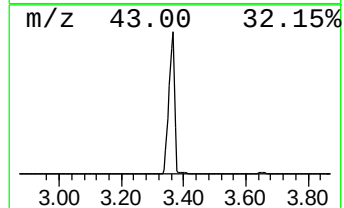
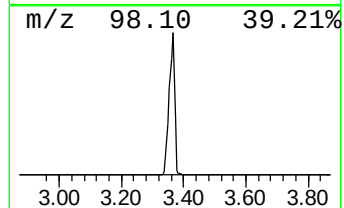
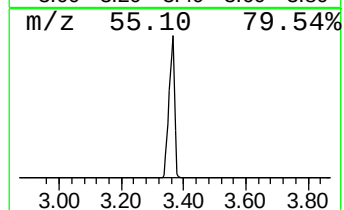
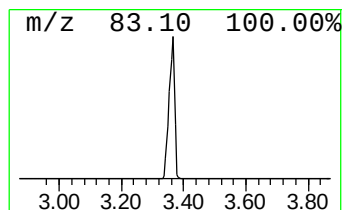
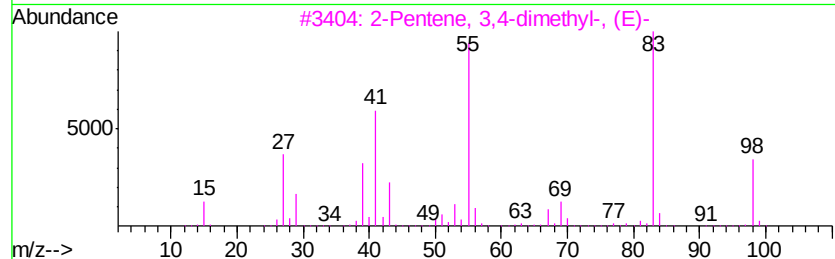
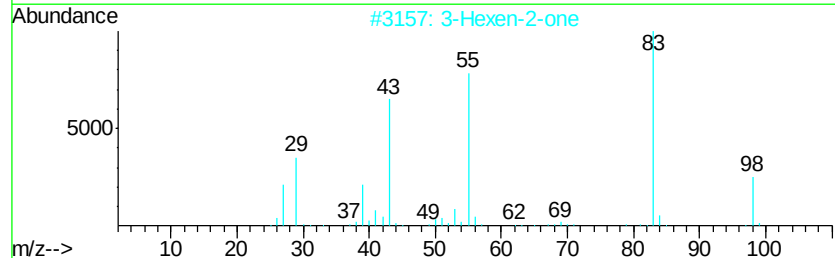
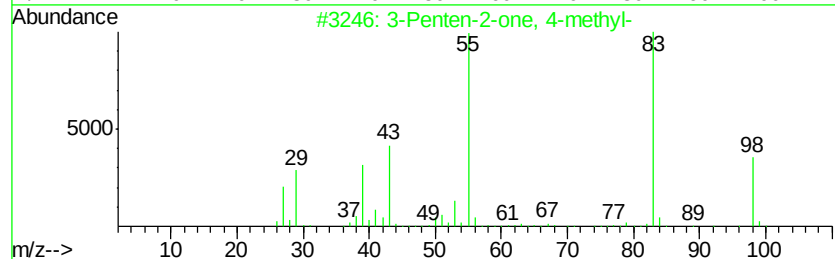
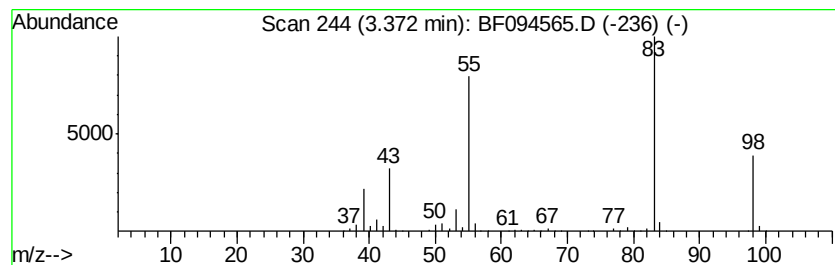
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.37	107.37 ng	3458700	1,4-Dichlorobenzene-d4	5.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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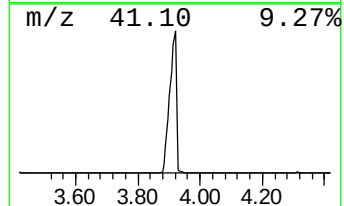
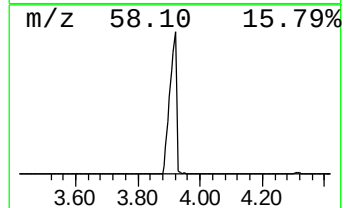
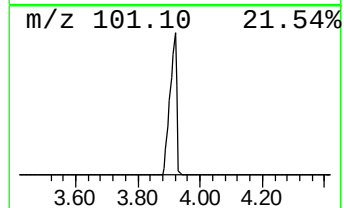
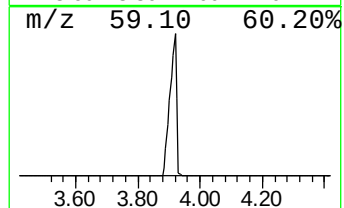
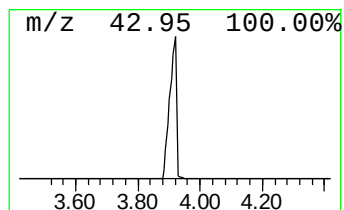
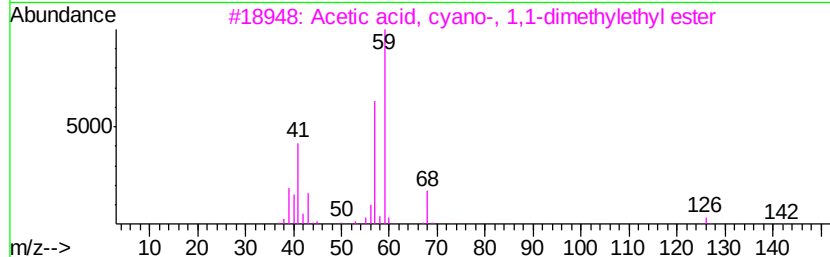
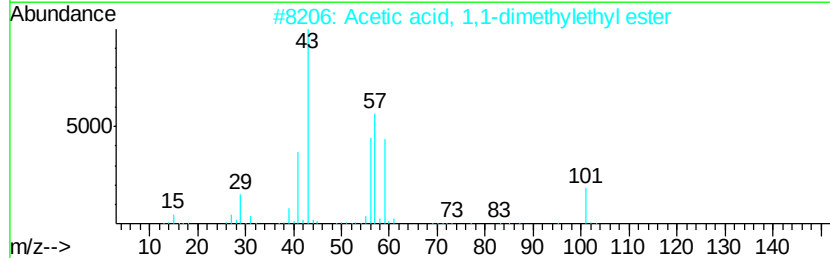
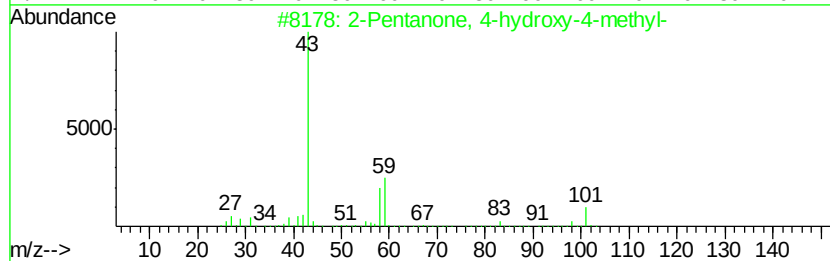
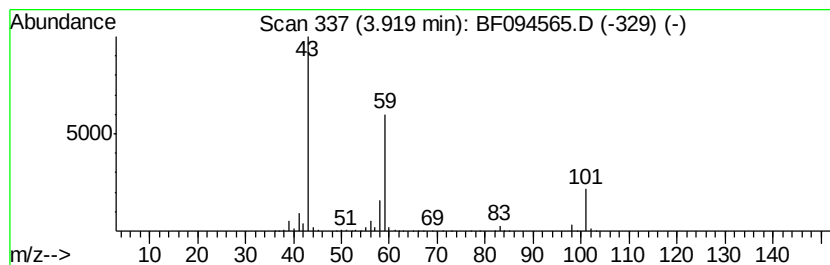
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.92	96.75 ng	3116350	1,4-Dichlorobenzene-d4	5.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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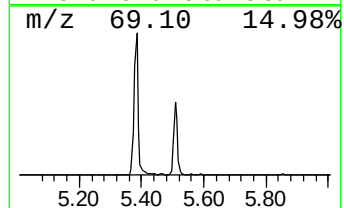
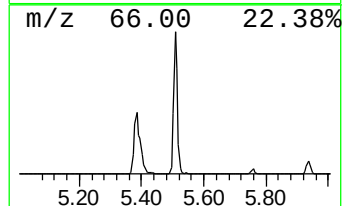
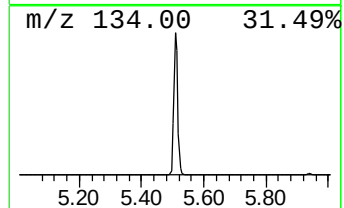
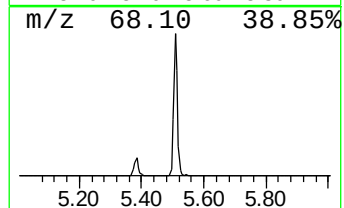
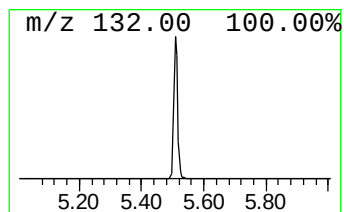
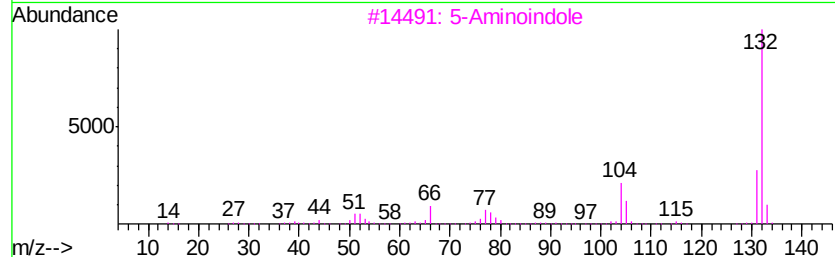
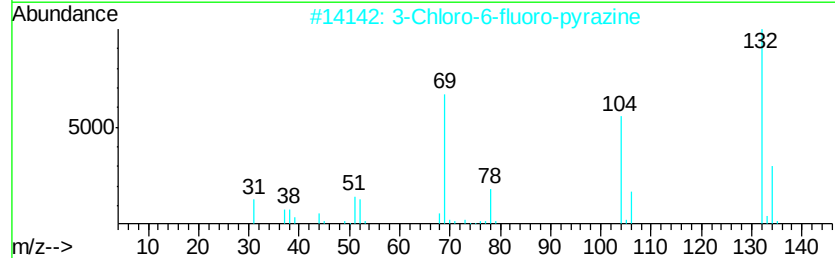
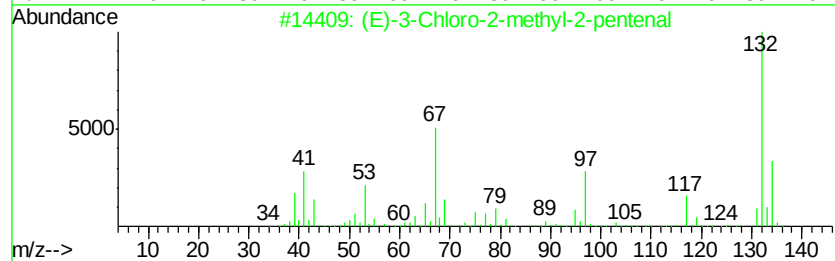
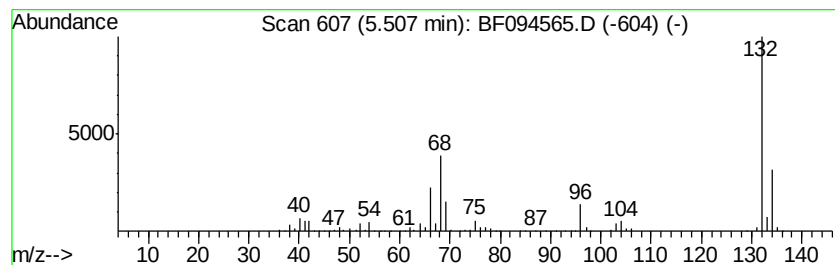
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown5.51 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.51	21.22 ng	683605	1,4-Dichlorobenzene-d4	5.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		Tranlycypromine-propionyl	189	C12H15NO	1000123-86-3	10



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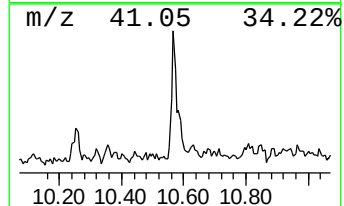
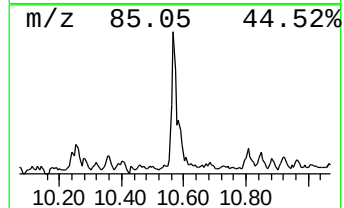
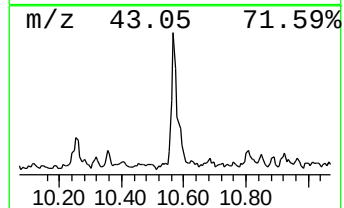
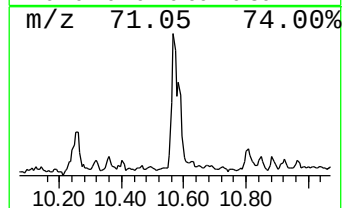
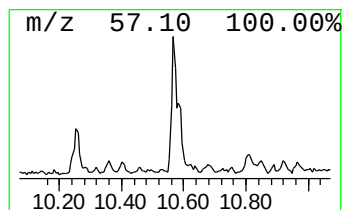
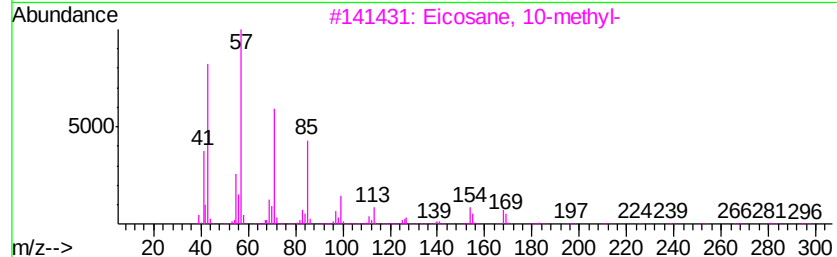
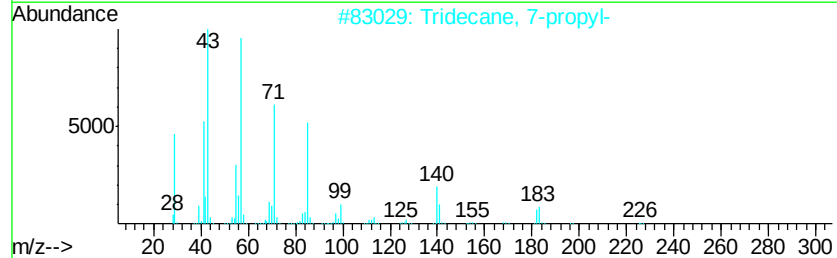
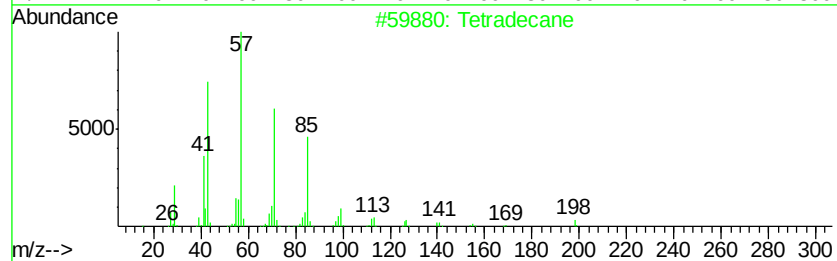
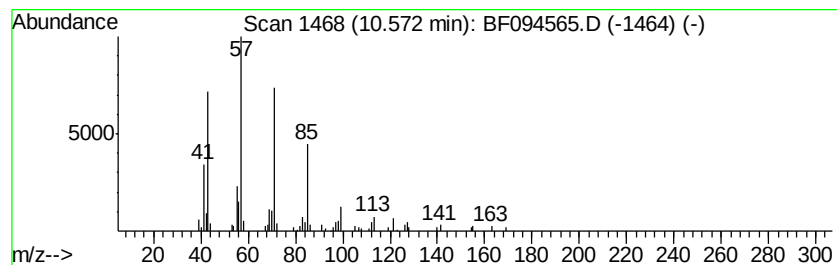
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C-9

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.57	2.49 ng	120503	Phenanthrene-d10	11.21	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	87
2	Tridecane, 7-propyl-	226	C16H34	055045-09-5	86
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	86
4	9-methylheptadecane	254	C18H38	026741-18-4	86
5	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	86



Data Path : Z:\HPCHEM1\BNA F\Data\BF042117\
Data File : BF094565.D
Acq On : 21 Apr 2017 16:27
Operator : SJ/MA
Sample : I2783-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

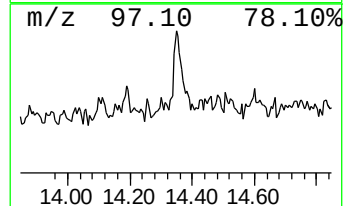
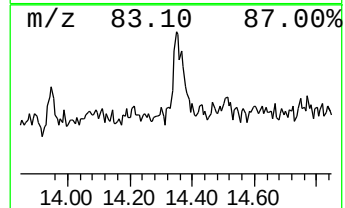
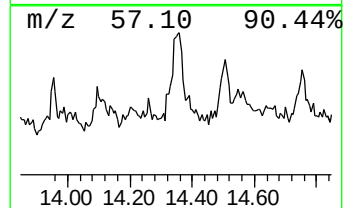
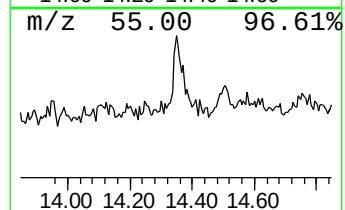
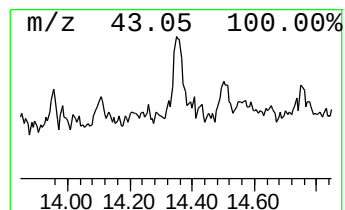
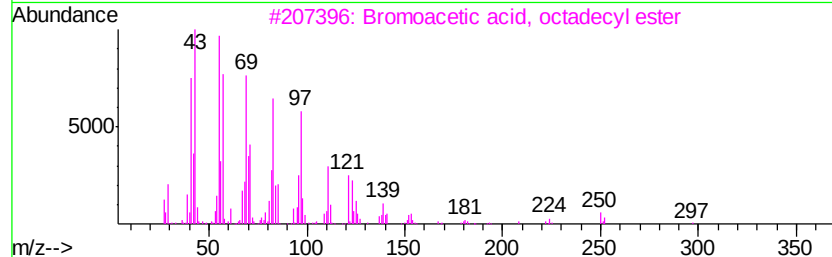
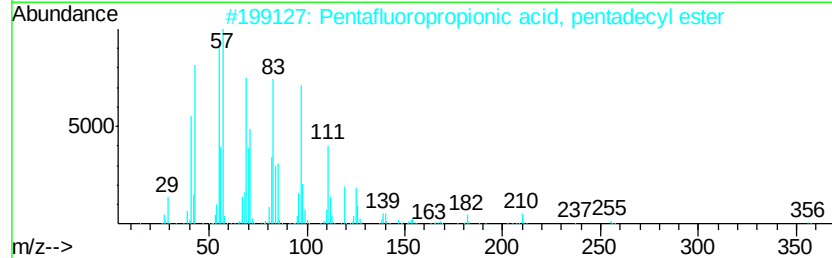
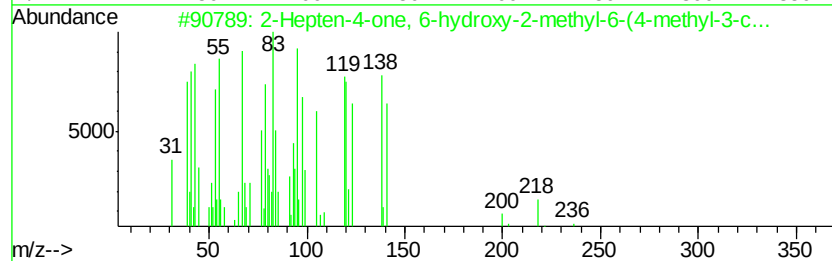
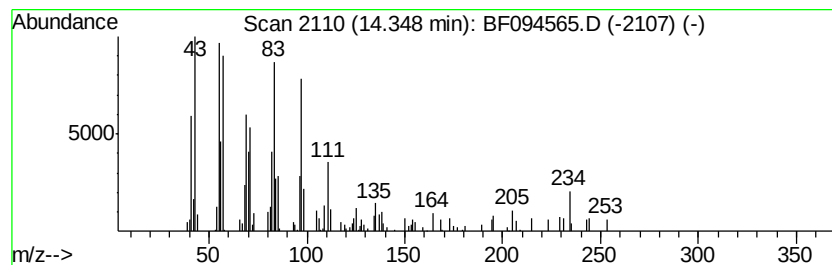
Instrument :
BNA_F
ClientSampled :
C-9

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-Hepten-4-one, 6-hydroxy-2... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.35	3.05 ng	125575	Chrysene-d12	14.45		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hepten-4-one, 6-hydroxy-2-meth...	236	C15H24O2	038043-98-0	91	
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	87	
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	87	
4	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	87	
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87	



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Data File : BF094565.D
Acq On : 21 Apr 2017 16:27
Operator : SJ/MA
Sample : I2783-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

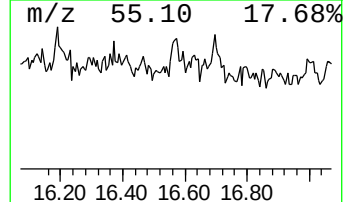
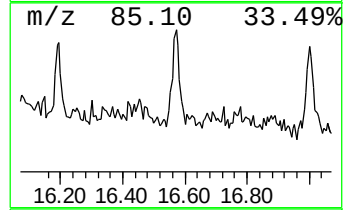
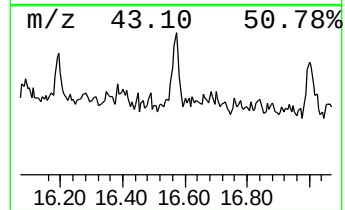
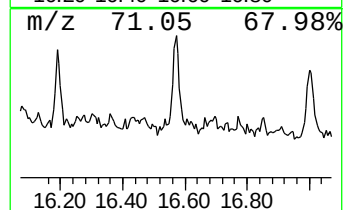
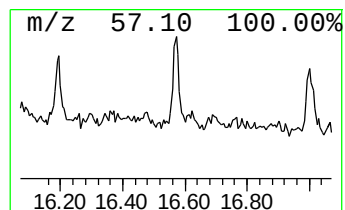
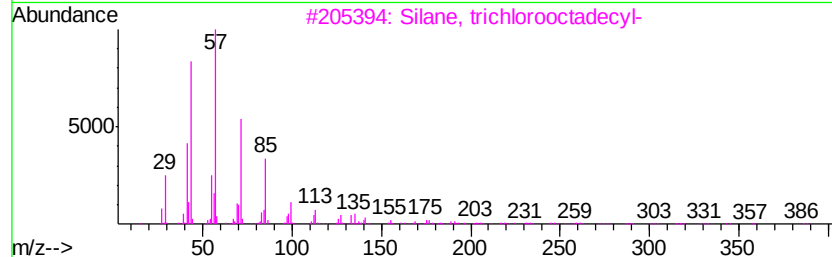
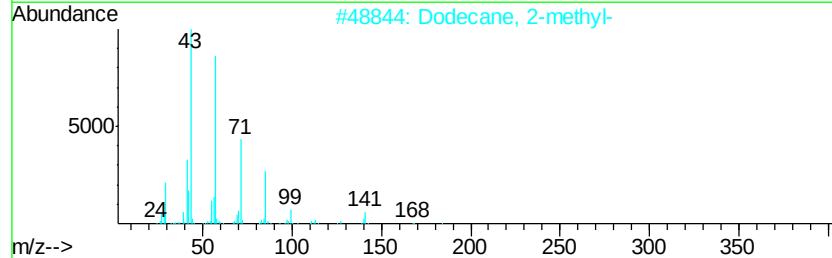
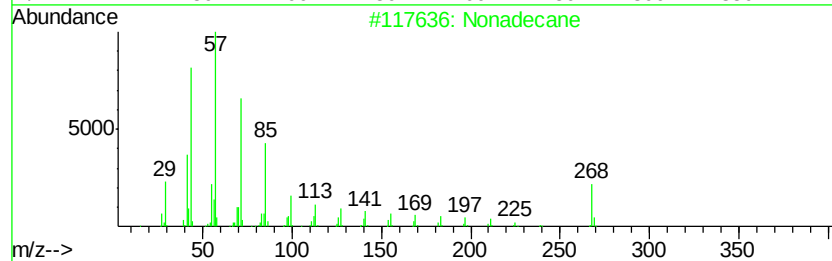
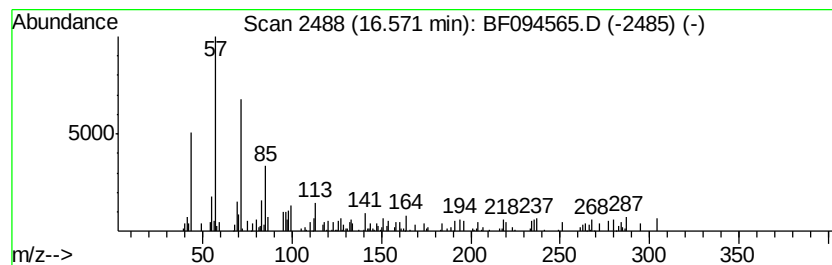
Instrument :
BNA_F
ClientSampleId :
C-9

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.57	2.23 ng	78875	Perylene-d12	16.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Nonadecane		268 C19H40	000629-92-5 64
2	Dodecane, 2-methyl-		184 C13H28	001560-97-0 47
3	Silane, trichlorooctadecyl-		386 C18H37Cl3Si	000112-04-9 47
4	Tetradecane, 2-methyl-		212 C15H32	001560-95-8 47
5	Tetratriacontane		479 C34H70	014167-59-0 47



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Sample : I2783-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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
4-Penten-2-one, 4...	2.70	2.5	ng	79539	1	5.76	644237	20.0
3-Penten-2-one, 4...	3.37	107.4	ng	3458700	1	5.76	644237	20.0
2-Pentanone, 4-hy...	3.92	96.8	ng	3116350	1	5.76	644237	20.0
unknown5.51	5.51	21.2	ng	683605	1	5.76	644237	20.0
Tetradecane	10.57	2.5	ng	120503	4	11.21	968352	20.0
2-Hepten-4-one, 6...	14.35	3.0	ng	125575	5	14.45	824442	20.0
Nonadecane	16.57	2.2	ng	78875	6	16.08	708452	20.0