

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081719\
 Data File : BF116362.D
 Acq On : 17 Aug 2019 17:26
 Operator : HP/JU
 Sample : K4391-06
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 N-WALL-0

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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	4.457	398	403	411	rBB2	58647	81690	3.25%	0.326%
2	4.869	465	473	477	rBV	54803	67588	2.69%	0.270%
3	4.945	482	486	494	rVB2	40956	59185	2.36%	0.236%
4	5.016	494	498	503	rBV2	30690	39189	1.56%	0.157%
5	5.222	529	533	536	rBV	72249	74670	2.97%	0.298%
6	5.434	566	569	578	rBV	1568681	1900778	75.68%	7.593%
7	5.581	590	594	599	rVB2	32848	44404	1.77%	0.177%
8	5.834	630	637	641	rBV2	59228	102785	4.09%	0.411%
9	5.881	641	645	648	rBV3	26177	37742	1.50%	0.151%
10	5.963	656	659	663	rVB2	57939	60879	2.42%	0.243%
11	6.010	663	667	670	rBV2	30249	37190	1.48%	0.149%
12	6.057	672	675	681	rVV2	78657	94177	3.75%	0.376%
13	6.116	681	685	687	rVV	51856	45911	1.83%	0.183%
14	6.245	702	707	710	rBV3	43506	53465	2.13%	0.214%
15	6.339	720	723	726	rBV2	43418	51418	2.05%	0.205%
16	6.451	738	742	755	rBV	1967810	2311043	92.02%	9.231%
17	6.581	761	764	772	rVB	2481176	2242605	89.29%	8.958%
18	6.810	800	803	811	rBV	931279	862844	34.35%	3.447%
19	6.963	826	829	840	rBV	1909531	1777859	70.79%	7.102%
20	7.375	896	899	917	rBV	1243688	1436583	57.20%	5.738%
21	8.086	1017	1020	1039	rBV	1071601	1160177	46.19%	4.634%
22	9.157	1199	1202	1214	rBV	2679948	2511571	100.00%	10.032%
23	9.557	1267	1270	1283	rBV	182848	180157	7.17%	0.720%
24	9.839	1314	1318	1336	rBV	1519657	1356975	54.03%	5.420%
25	10.633	1449	1453	1468	rBV	1340094	1526193	60.77%	6.096%
26	11.327	1568	1571	1580	rBV	1471364	1364185	54.32%	5.449%
27	11.392	1580	1582	1587	rVB2	35684	36243	1.44%	0.145%
28	11.851	1657	1660	1674	rBV2	34179	59625	2.37%	0.238%
29	12.368	1739	1748	1751	rBV2	22214	40146	1.60%	0.160%
30	12.398	1751	1753	1765	rVB	42478	53657	2.14%	0.214%
31	12.904	1835	1839	1849	rBV	2801852	2456574	97.81%	9.813%
32	13.127	1870	1877	1887	rBV	48839	55067	2.19%	0.220%
33	13.792	1986	1990	2007	rBV2	197625	413891	16.48%	1.653%
34	13.968	2016	2020	2032	rBV	1124959	1116488	44.45%	4.460%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.409	2092	2095	2098	rBV	33200	40195	1.60%	0.161%
36	14.709	2142	2146	2150	rBV	39061	41372	1.65%	0.165%
37	14.786	2155	2159	2162	rBV	106518	98301	3.91%	0.393%
38	15.039	2198	2202	2207	rBV	41498	51009	2.03%	0.204%
39	15.421	2259	2267	2285	rBV	663297	998500	39.76%	3.988%
40	15.821	2330	2335	2339	rVB	30375	43558	1.73%	0.174%
41	16.303	2412	2417	2429	rVB3	22403	48774	1.94%	0.195%

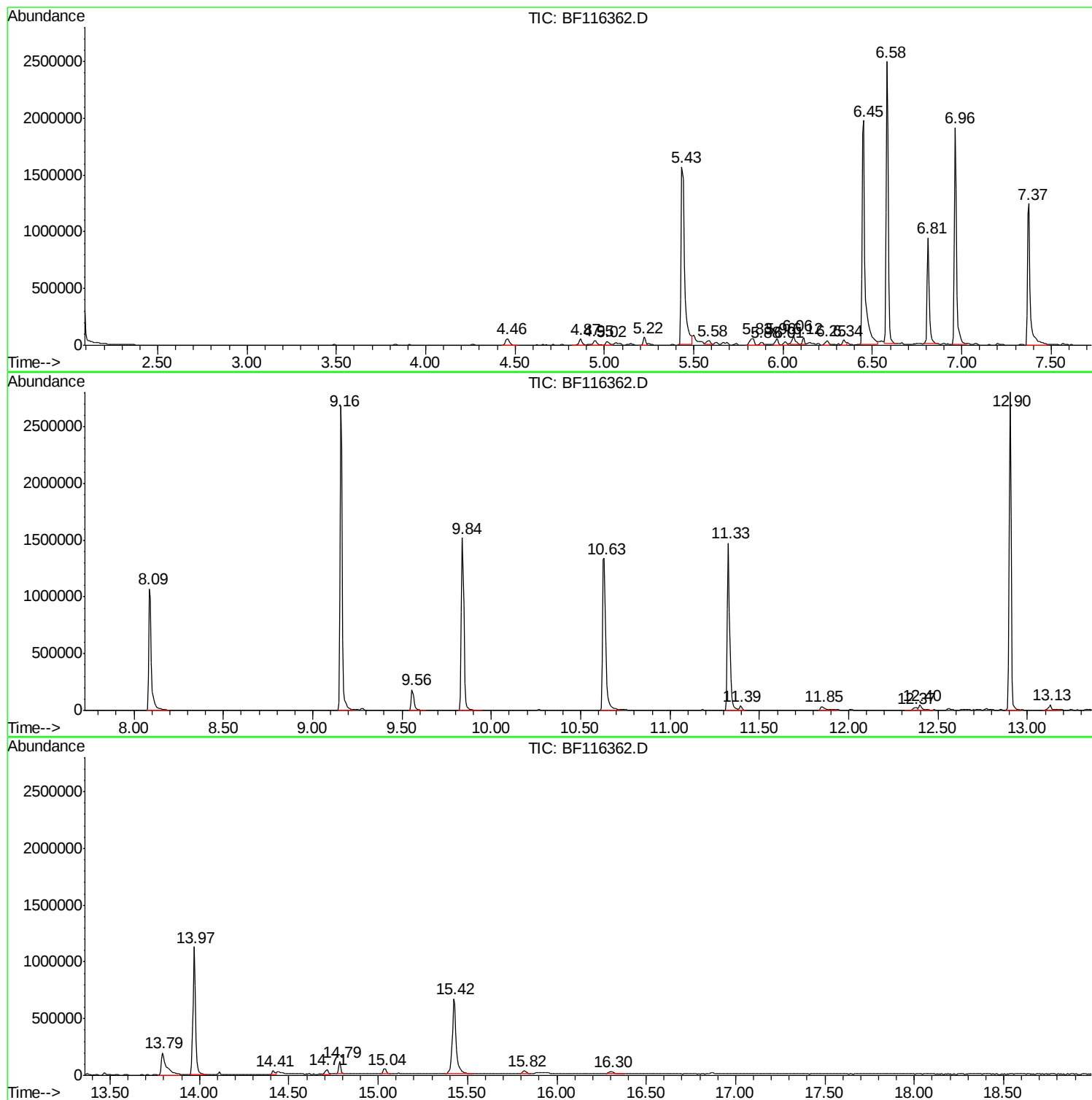
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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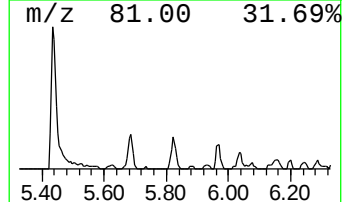
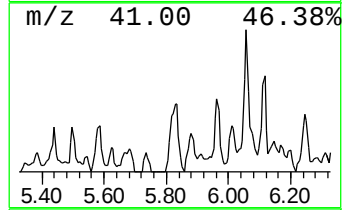
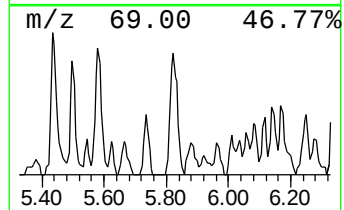
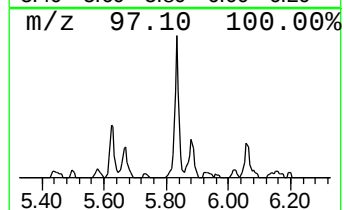
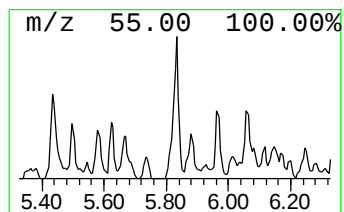
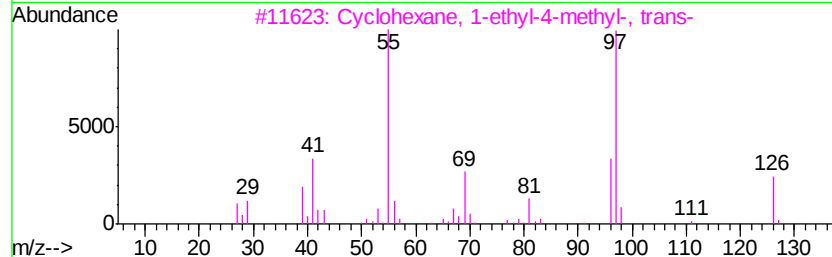
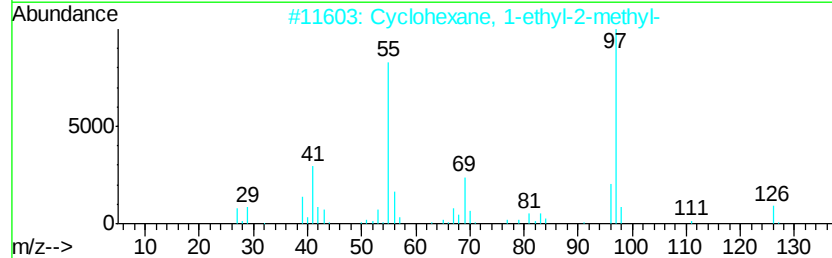
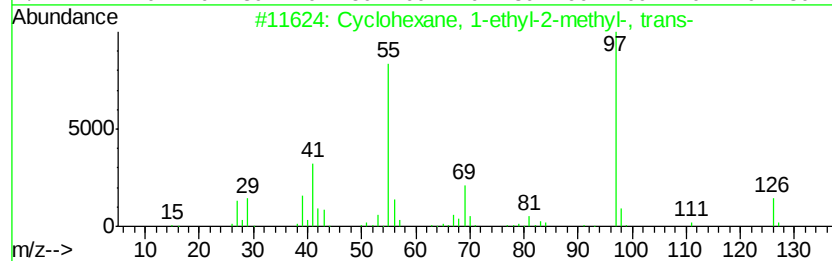
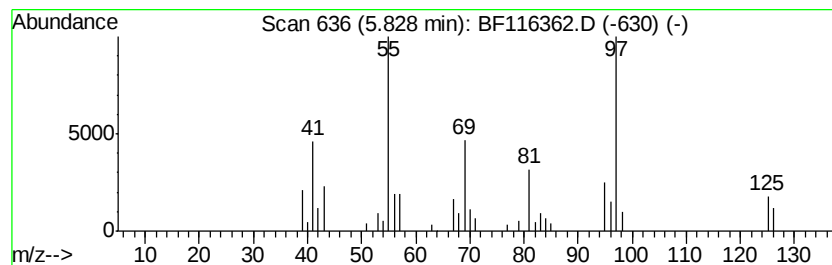
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclohexane, 1-ethyl-2-meth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.83	2.38 ng	102785	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	87
2			Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	87
3			Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	86
4			1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	86
5			cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	86



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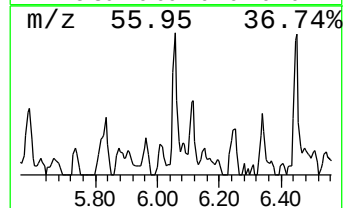
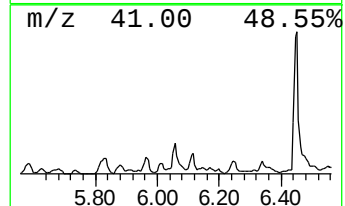
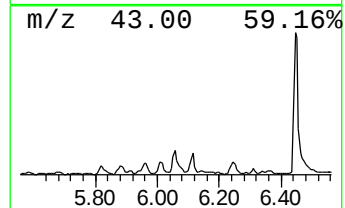
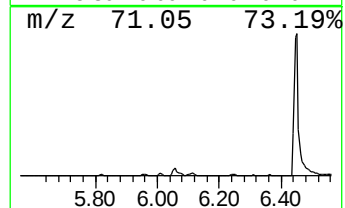
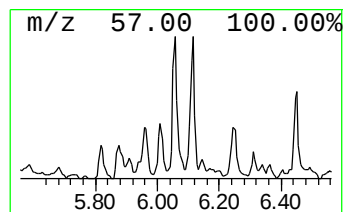
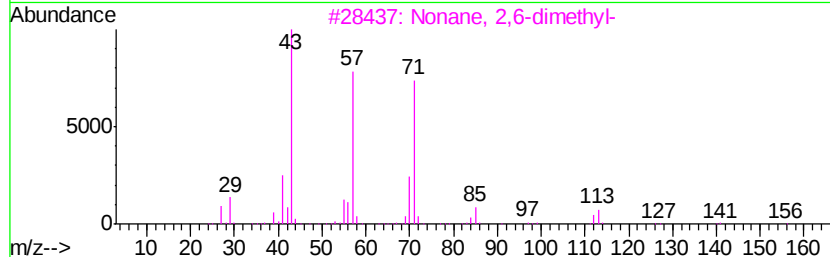
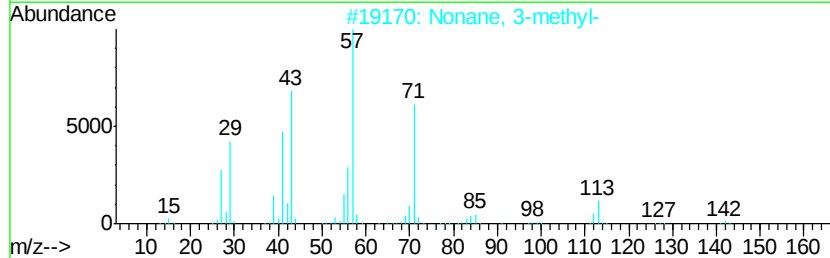
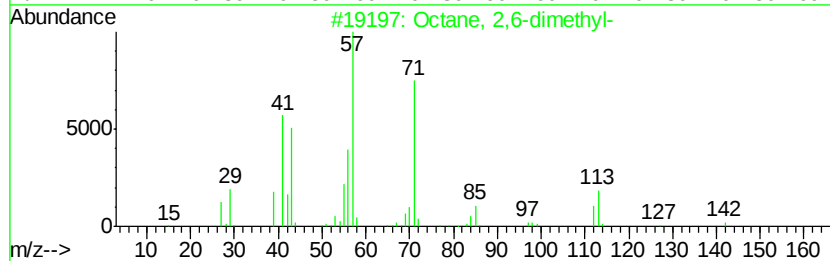
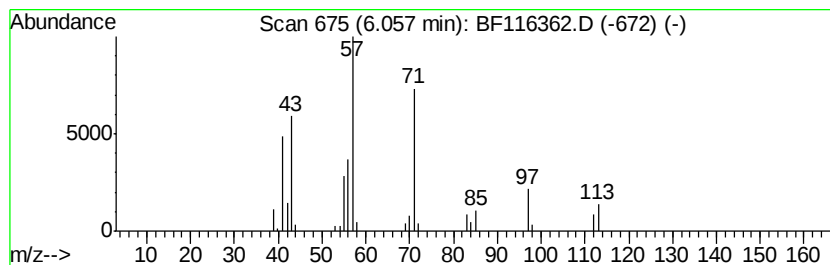
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Peak Number 2 Octane, 2,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.06	2.18 ng	94177	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	78
2		Nonane, 3-methyl-	142	C10H22	005911-04-6	72
3		Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	64
4		Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	64
5		Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	59



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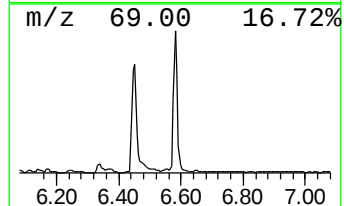
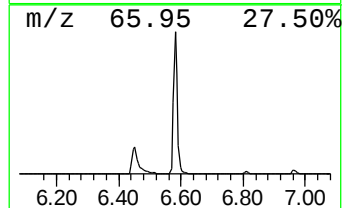
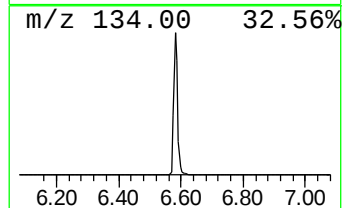
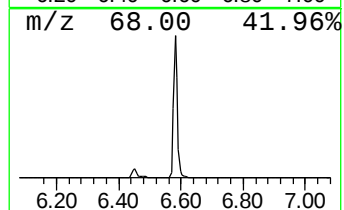
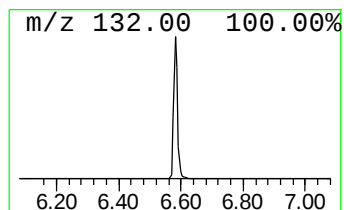
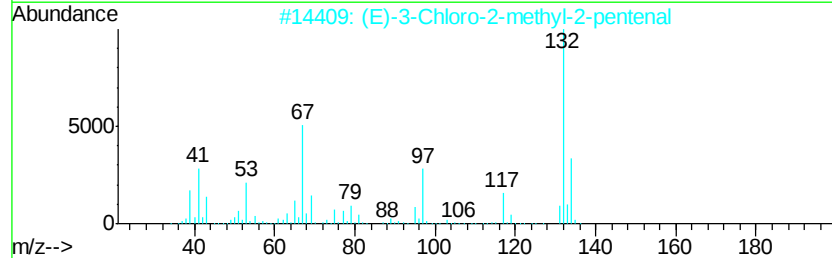
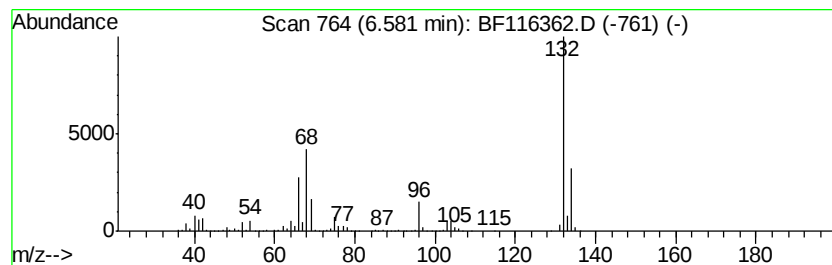
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	51.98 ng	2242610	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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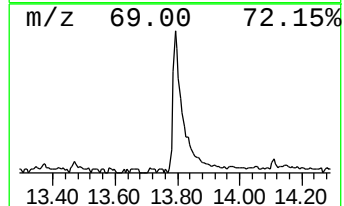
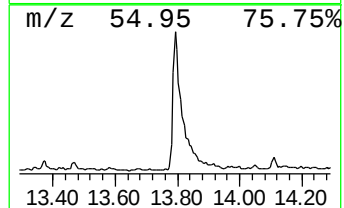
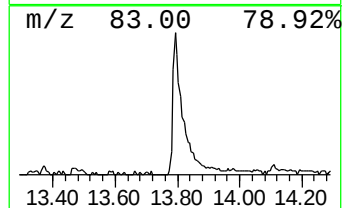
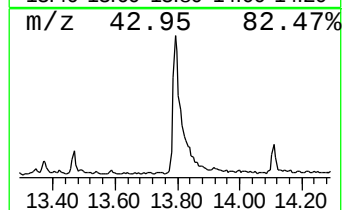
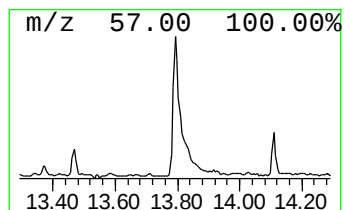
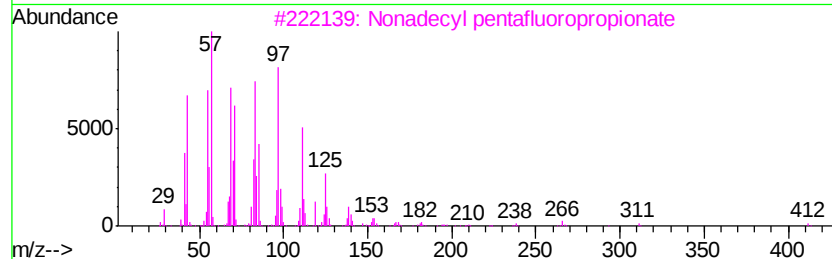
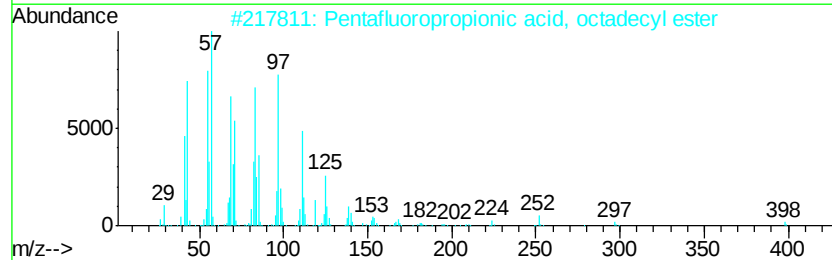
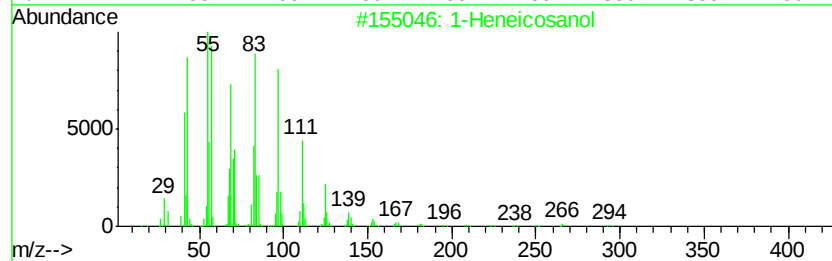
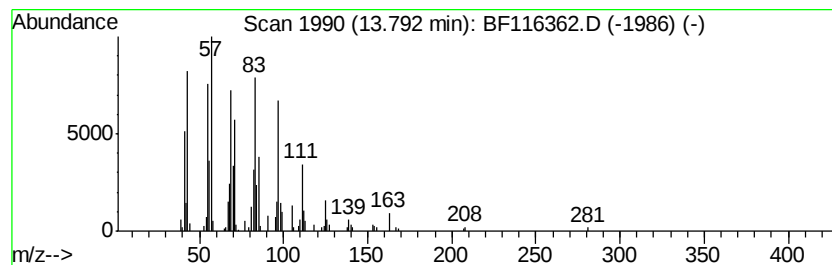
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	7.41 ng	413891	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	93
2		Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	91
3		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4		1-Heptacosanol	396	C27H56O	002004-39-9	90
5		Pentafluoropropionic acid, heptadecyl ester	402	C20H35F5O2	959218-78-1	90



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexane, 1-et...	5.83	2.4	ng	102785	1	6.81	862844	20.0
Octane, 2,6-dimet...	6.06	2.2	ng	94177	1	6.81	862844	20.0
unknown6.58	6.58	52.0	ng	2242610	1	6.81	862844	20.0
1-Heneicosanol	13.79	7.4	ng	413891	5	13.97	1116490	20.0