

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120817\
 Data File : BF101276.D
 Acq On : 9 Dec 2017 11:07
 Operator : SJ/JU
 Sample : I6744-09
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PROS-1-E(0-1)

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-BF113017.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	5.051	501	504	515	rBB	39056	50525	5.28%	0.534%
2	5.451	568	572	586	rBV	935051	885010	92.43%	9.355%
3	6.475	741	746	764	rBV	862448	957441	100.00%	10.121%
4	6.604	764	768	771	rBV	1129602	921447	96.24%	9.740%
5	6.828	803	806	814	rBB	283062	240621	25.13%	2.544%
6	6.987	829	833	836	rBV	887631	719759	75.18%	7.608%
7	7.398	898	903	906	rBV	539946	478089	49.93%	5.054%
8	8.110	1021	1024	1032	rBV	313742	286245	29.90%	3.026%
9	9.186	1203	1207	1210	rBV	1147315	926196	96.74%	9.790%
10	9.257	1216	1219	1223	rVB	15073	13237	1.38%	0.140%
11	9.580	1268	1274	1277	rBV	74786	60951	6.37%	0.644%
12	9.786	1303	1309	1312	rBV	32919	28935	3.02%	0.306%
13	9.869	1320	1323	1327	rBV	319845	274890	28.71%	2.906%
14	10.286	1392	1394	1397	rVB	33976	28260	2.95%	0.299%
15	10.422	1413	1417	1421	rVB	14340	13991	1.46%	0.148%
16	10.663	1454	1458	1462	rBV	536482	459572	48.00%	4.858%
17	10.763	1471	1475	1480	rBV	31327	34064	3.56%	0.360%
18	11.210	1548	1551	1554	rBV	21886	18968	1.98%	0.201%
19	11.363	1573	1577	1579	rBV	347613	281478	29.40%	2.975%
20	11.386	1579	1581	1584	rVV	181726	135005	14.10%	1.427%
21	11.439	1587	1590	1593	rBV	64333	48714	5.09%	0.515%
22	11.639	1621	1624	1628	rVB3	10474	11945	1.25%	0.126%
23	11.863	1659	1662	1665	rBV	20878	27569	2.88%	0.291%
24	11.892	1665	1667	1671	rVB	35342	28891	3.02%	0.305%
25	11.939	1671	1675	1678	rVB	17662	16141	1.69%	0.171%
26	11.980	1678	1682	1684	rBV	44715	50026	5.22%	0.529%
27	12.157	1709	1712	1715	rBV	21039	17264	1.80%	0.182%
28	12.310	1732	1738	1741	rBV4	7448	15899	1.66%	0.168%
29	12.416	1751	1756	1758	rBV	18696	25730	2.69%	0.272%
30	12.504	1768	1771	1774	rBV4	9480	15034	1.57%	0.159%
31	12.580	1780	1784	1787	rBV	353916	287150	29.99%	3.035%
32	12.757	1811	1814	1817	rVB2	33800	28191	2.94%	0.298%
33	12.810	1817	1823	1829	rBV	288683	333627	34.85%	3.527%
34	12.863	1829	1832	1836	rVB3	15656	19104	2.00%	0.202%

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PROS-1-E(0-1)

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-BF113017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.945	1841	1846	1849	rBV	849977	782648	81.74%	8.273%
36	13.027	1856	1860	1864	rBV4	18827	32058	3.35%	0.339%
37	13.139	1876	1879	1882	rVB	45334	41083	4.29%	0.434%
38	13.204	1887	1890	1892	rBV	43305	39042	4.08%	0.413%
39	13.368	1915	1918	1922	rBV4	16991	22999	2.40%	0.243%
40	13.763	1983	1985	1987	rBV	24614	18550	1.94%	0.196%
41	13.833	1994	1997	2000	rVB2	69770	71099	7.43%	0.752%
42	13.974	2017	2021	2023	rBV	111919	116388	12.16%	1.230%
43	14.010	2023	2027	2030	rVV2	299685	367619	38.40%	3.886%
44	14.039	2030	2032	2035	rVB	101352	84524	8.83%	0.893%
45	15.492	2276	2279	2282	rVB2	133974	144249	15.07%	1.525%

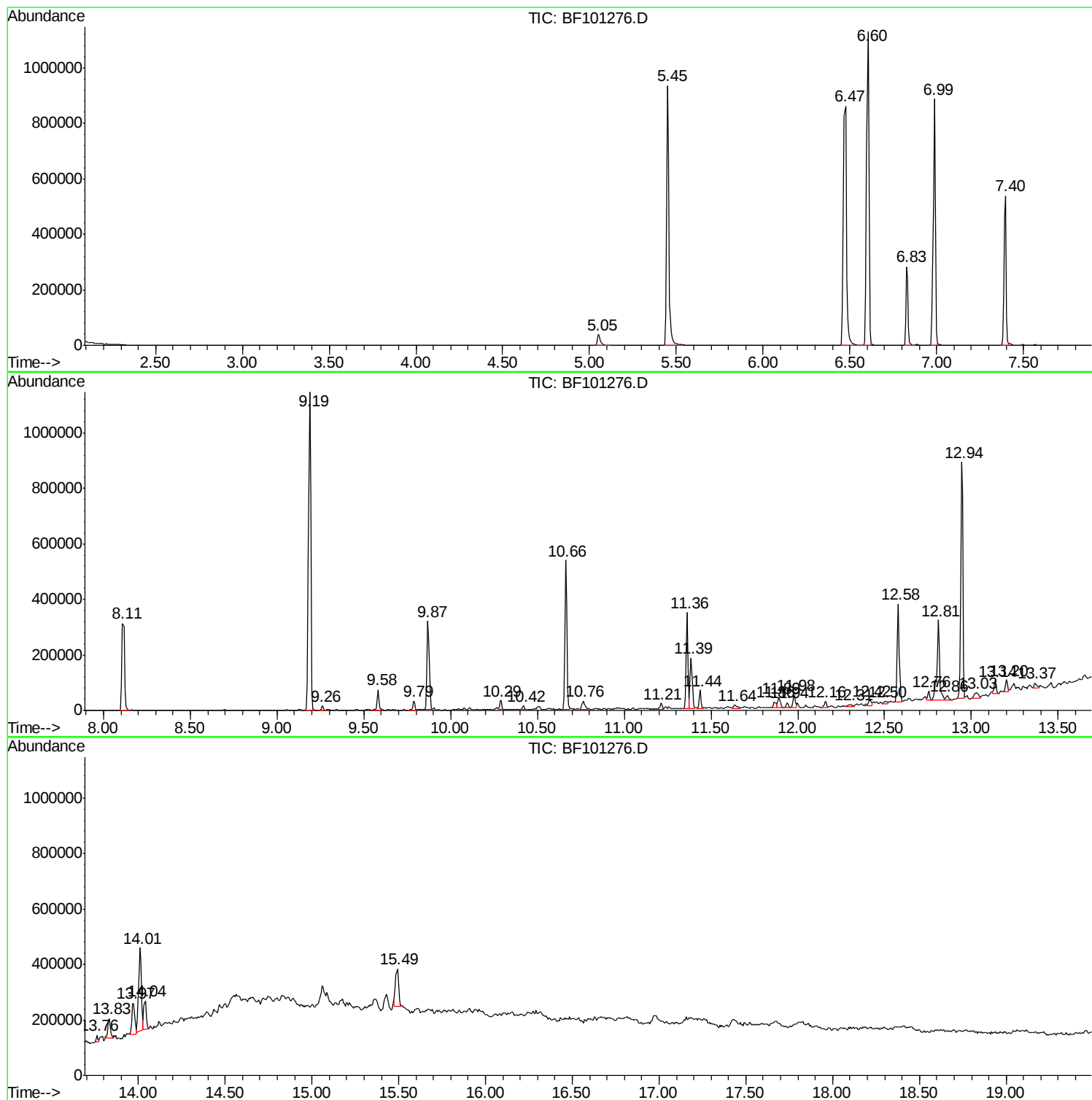
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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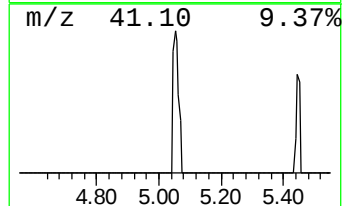
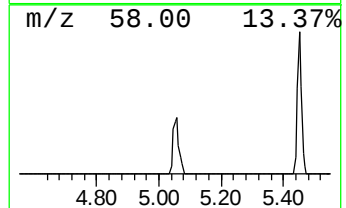
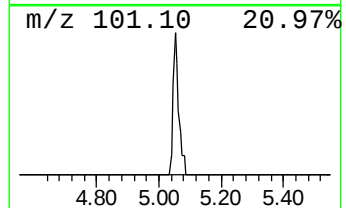
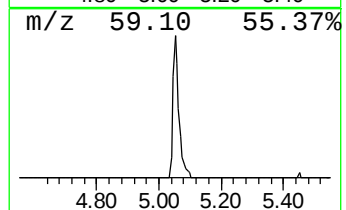
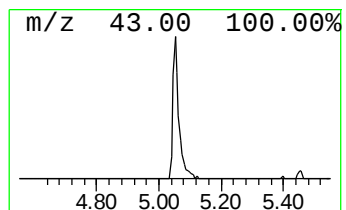
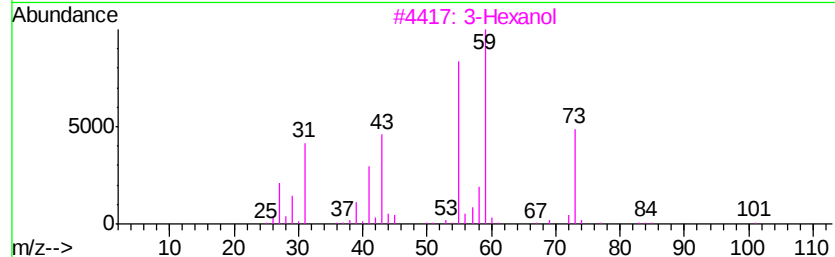
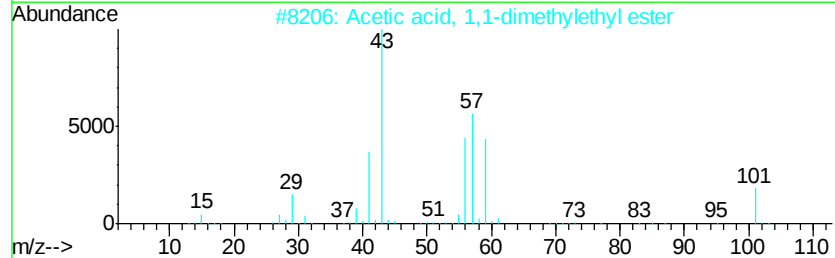
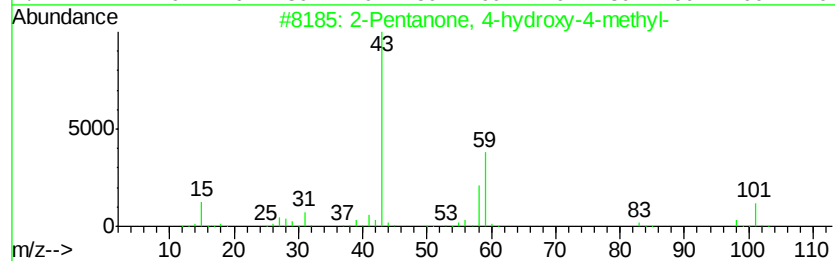
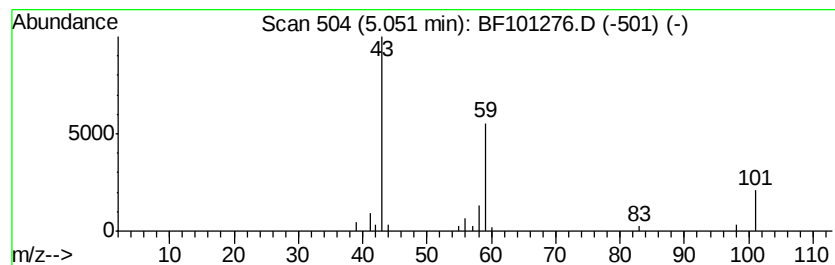
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.05	4.20 ng	50525	1,4-Dichlorobenzene-d4	6.83

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	40	
3	3-Hexanol	102	C6H14O	000623-37-0	33	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32	
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9	



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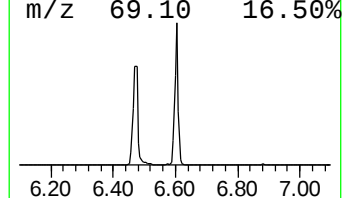
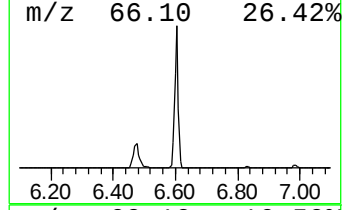
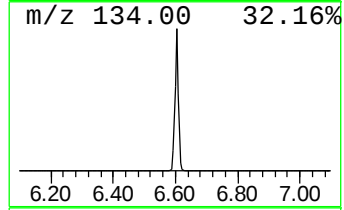
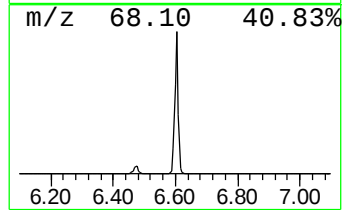
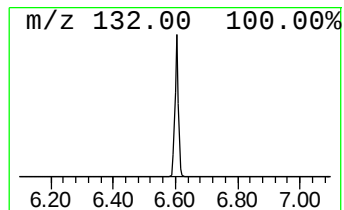
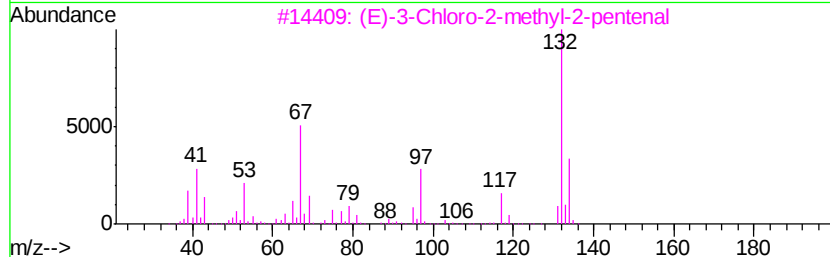
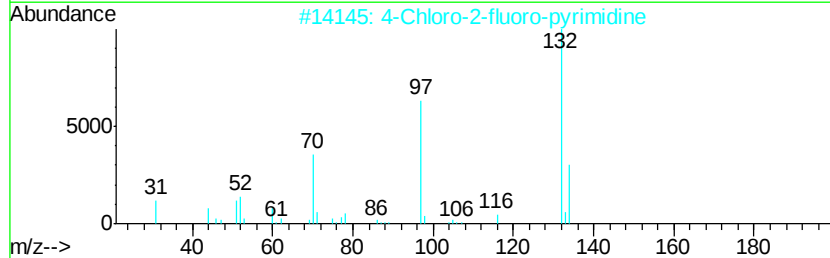
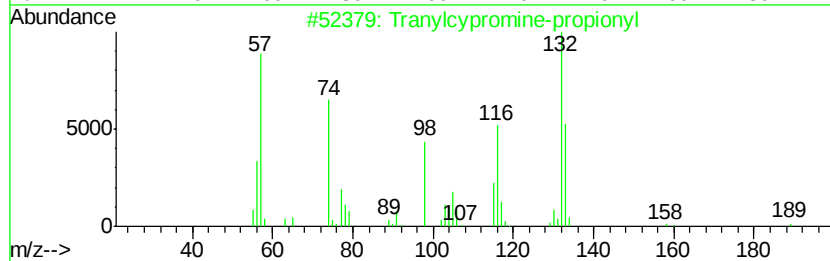
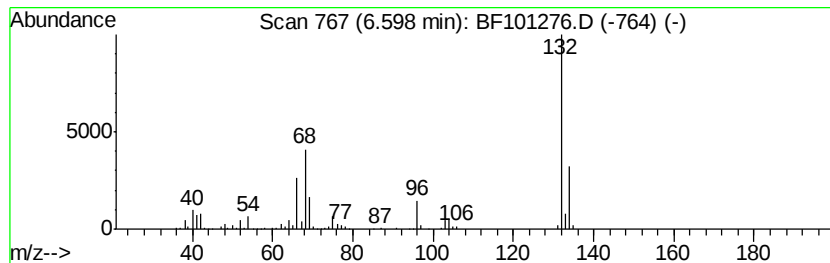
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Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	76.59 ng	921447	1,4-Dichlorobenzene-d4	6.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	10
2			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
3			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5			1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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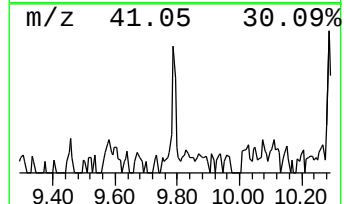
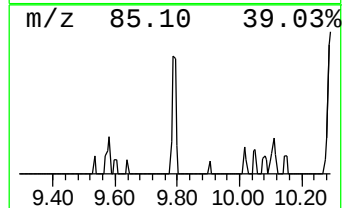
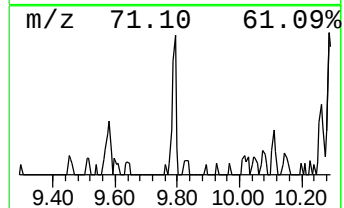
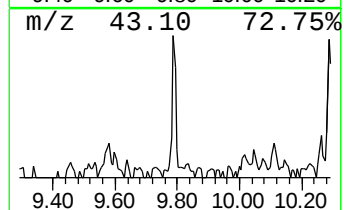
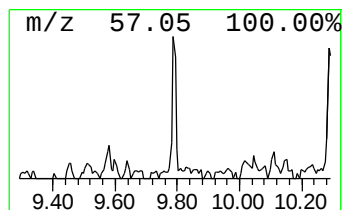
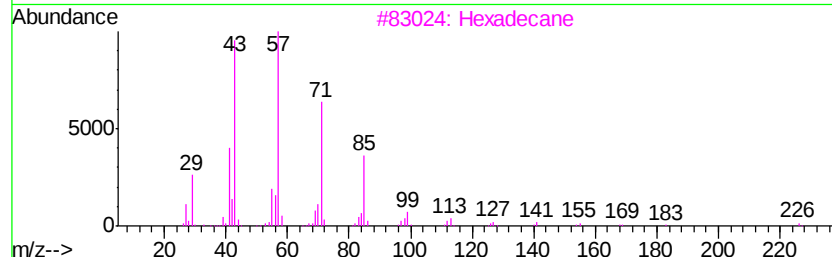
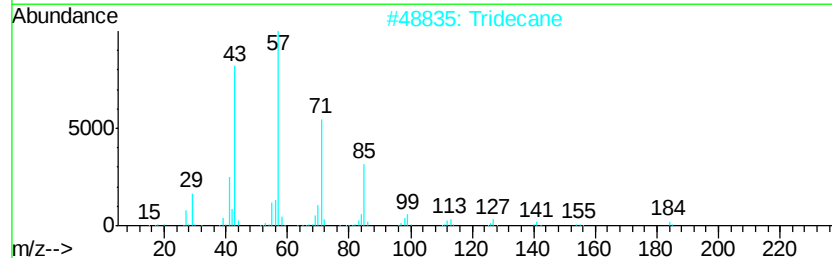
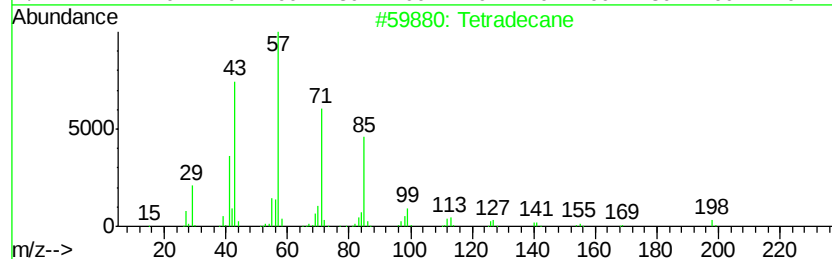
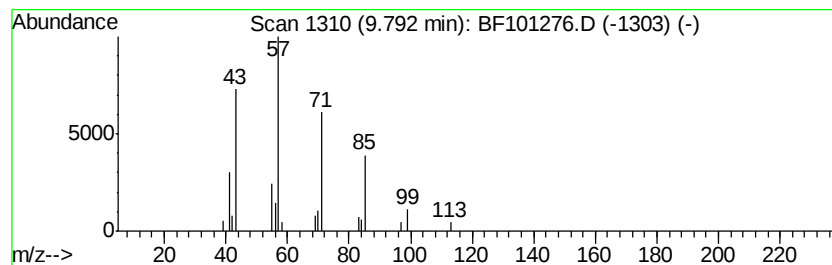
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.79	2.11 ng	28935	Acenaphthene-d10	9.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	83
2			Tridecane	184	C13H28	000629-50-5	83
3			Hexadecane	226	C16H34	000544-76-3	83
4			Pentadecane	212	C15H32	000629-62-9	83
5			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	78



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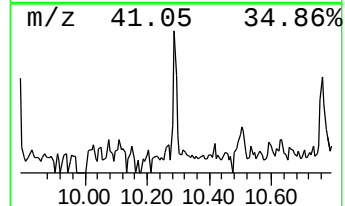
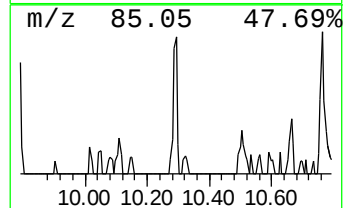
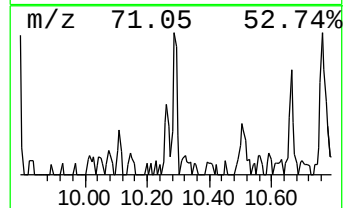
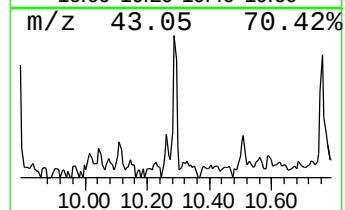
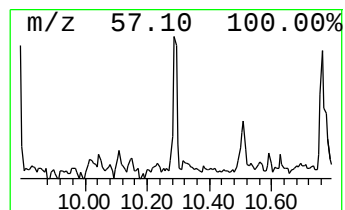
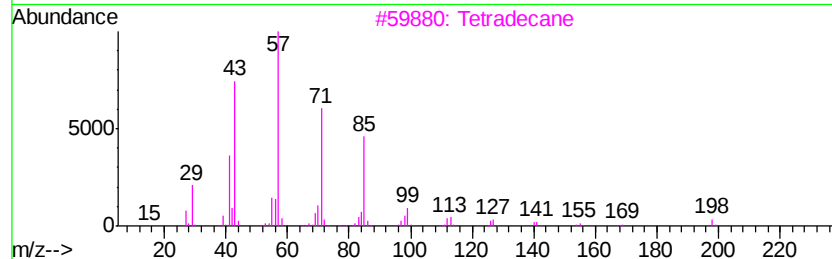
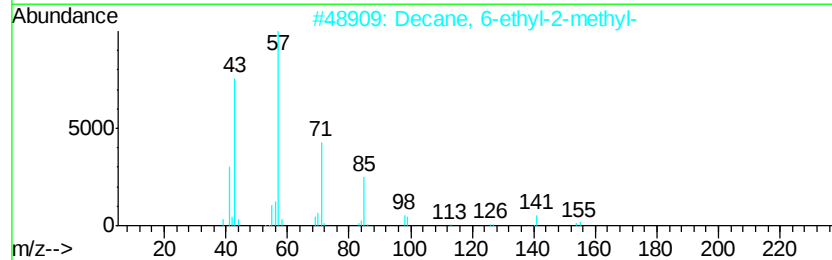
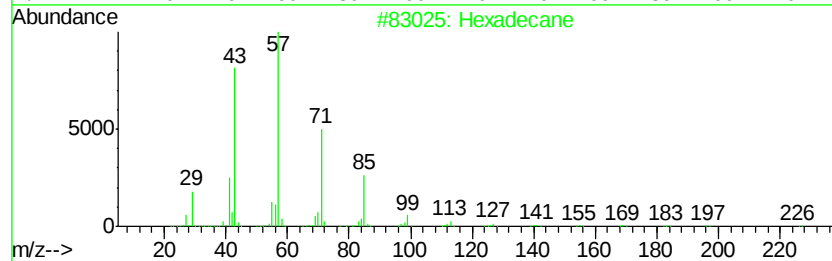
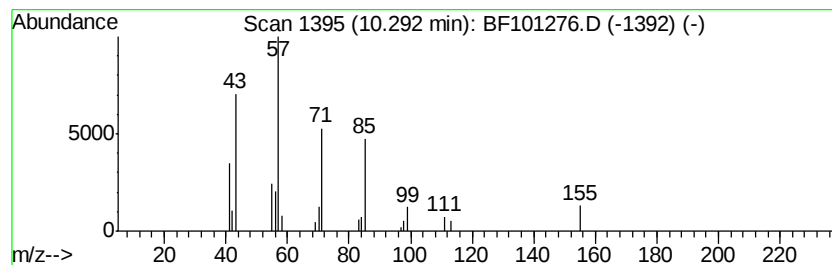
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.29	2.06 ng	28260	Acenaphthene-d10	9.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	83
2		Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	83
3		Tetradecane	198	C14H30	000629-59-4	83
4		Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	72
5		1-Iodoundecane	282	C11H23I	004282-44-4	72



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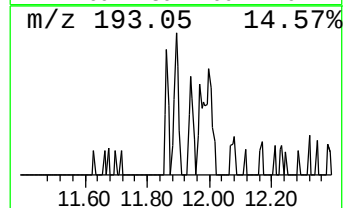
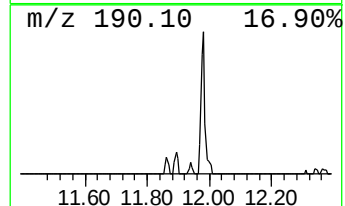
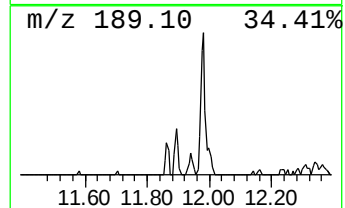
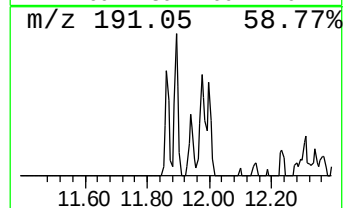
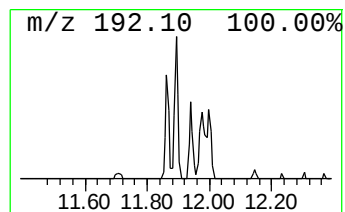
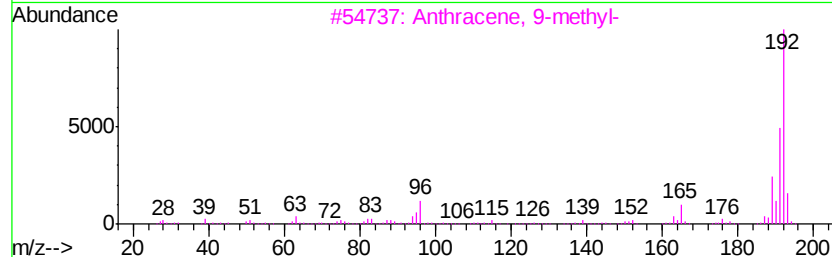
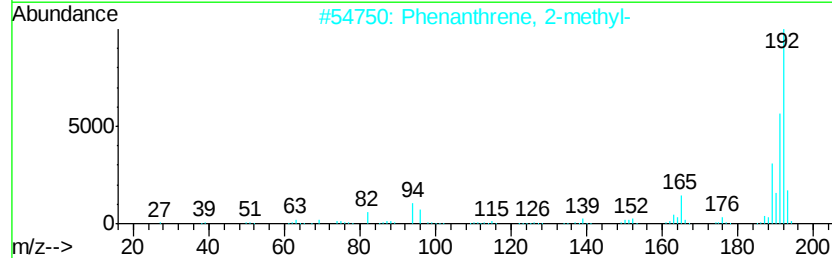
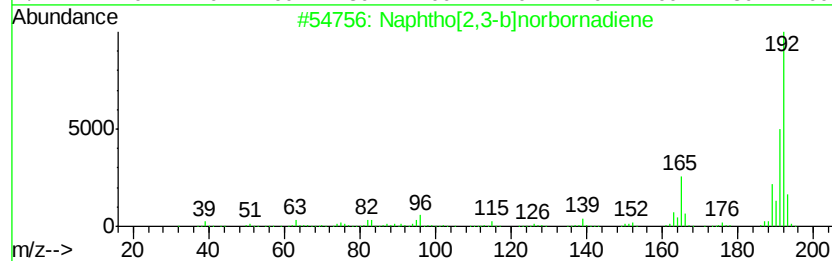
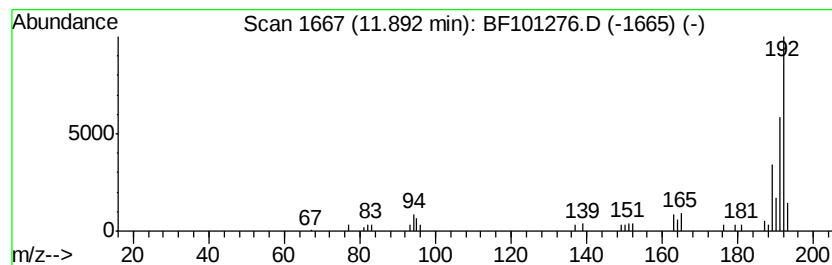
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Naphtho[2,3-b]norbornadiene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	2.05 ng	28891	Phenanthrene-d10	11.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	87
2		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	87
3		Anthracene, 9-methyl-	192	C15H12	000779-02-2	87
4		Anthracene, 1-methyl-	192	C15H12	000610-48-0	87
5		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120817\
Data File : BF101276.D
Acq On : 9 Dec 2017 11:07
Operator : SJ/JU
Sample : I6744-09
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PROS-1-E(0-1)

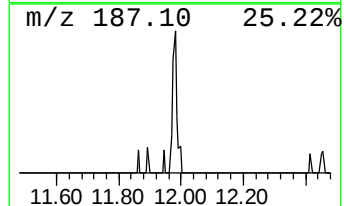
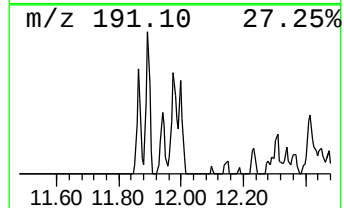
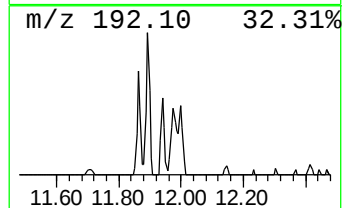
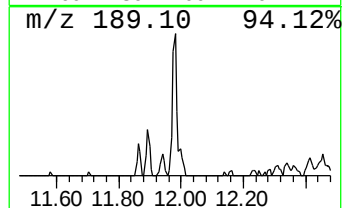
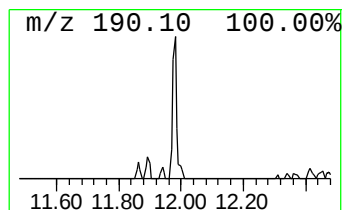
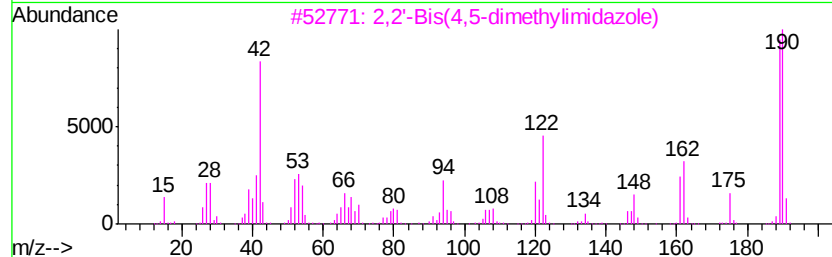
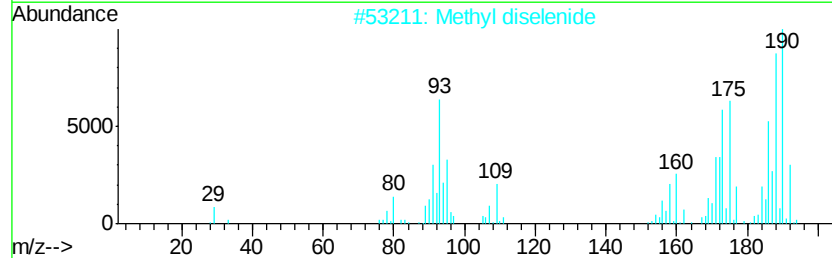
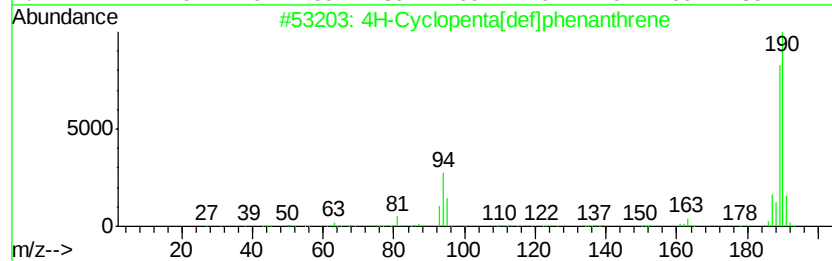
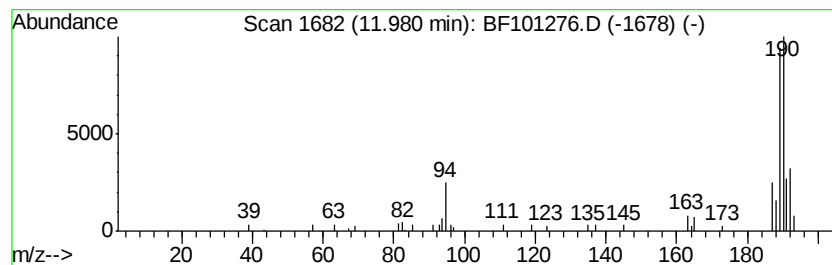
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.98	3.55 ng	50026	Phenanthrene-d10	11.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	72
2		Methyl diselenide	190	C2H6Se2	007101-31-7	43
3		2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42
4		Benzimidazol-2(3H)-one, 5-formyl...	190	C10H10N2O2	055241-49-1	33
5		1H-Pyrazole-4-carboxaldehyde, 1-...	190	C10H7FN2O	1000338-05-6	28



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Sample : I6744-09
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PROS-1-E(0-1)

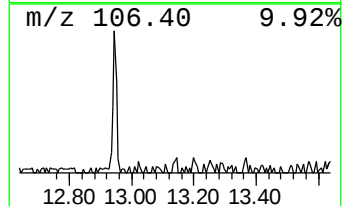
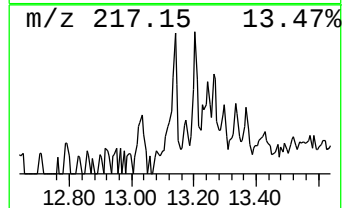
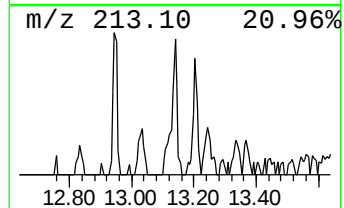
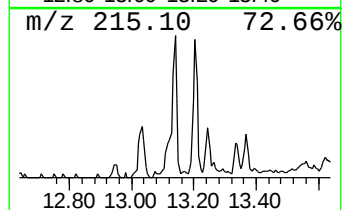
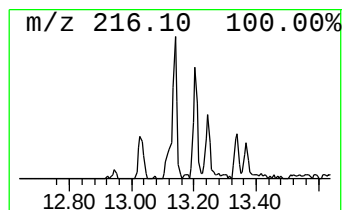
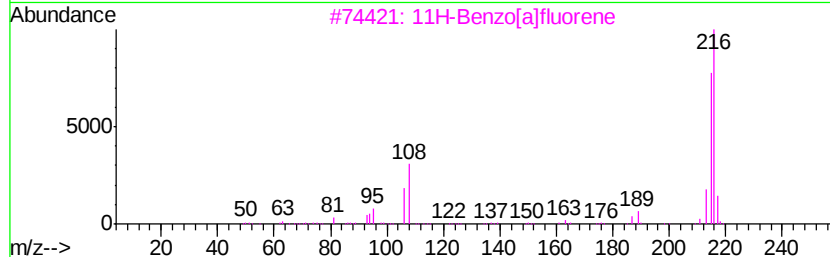
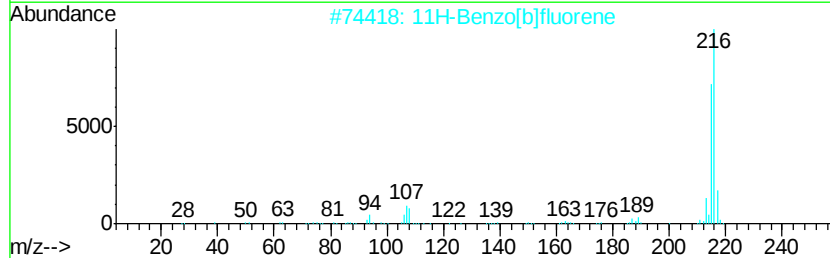
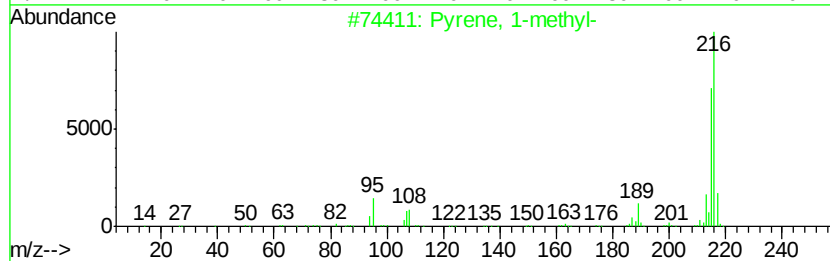
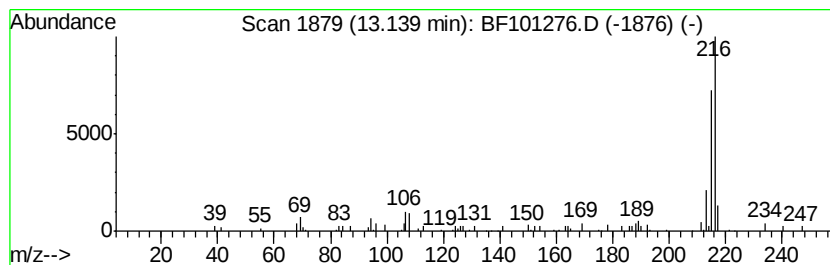
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.14	2.24 ng	41083	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	83
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	72
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	72
4	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	59
5	trans-p-(Trifluoromethyl)cinnami...	216	C10H7F3O2	016642-92-5	53



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Sample : I6744-09
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PROS-1-E(0-1)

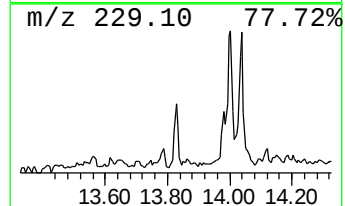
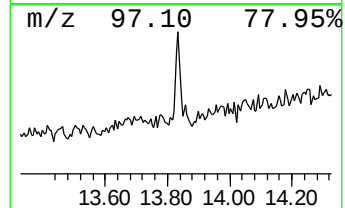
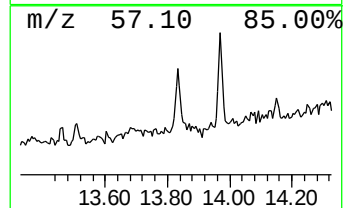
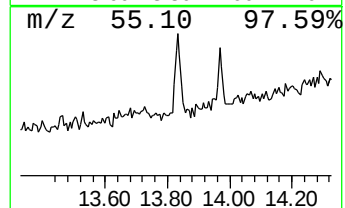
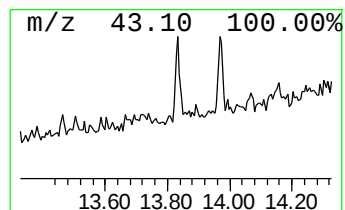
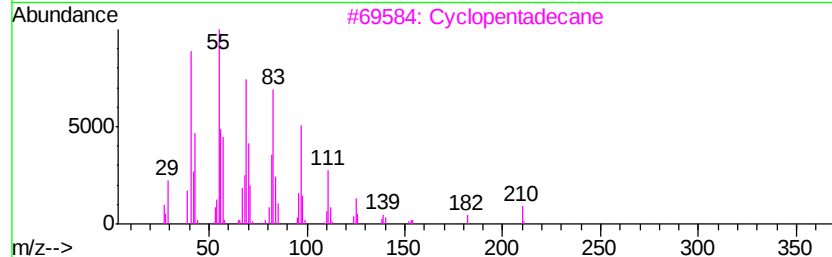
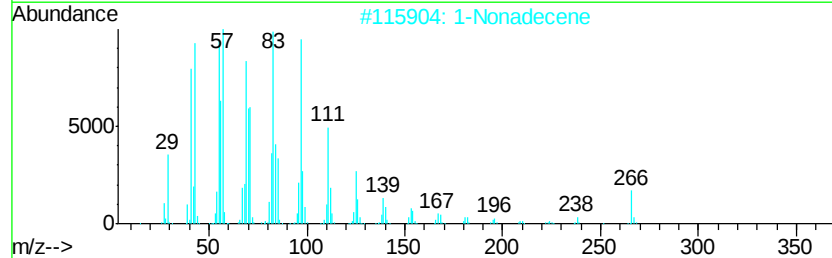
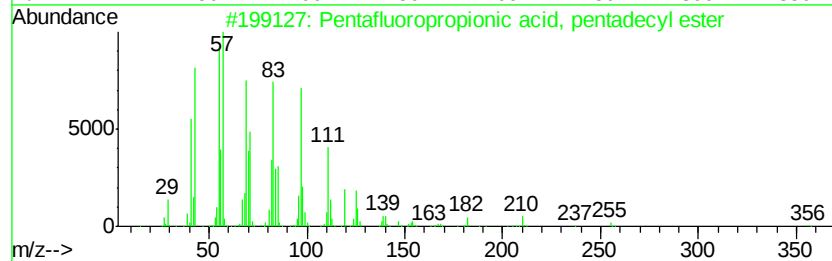
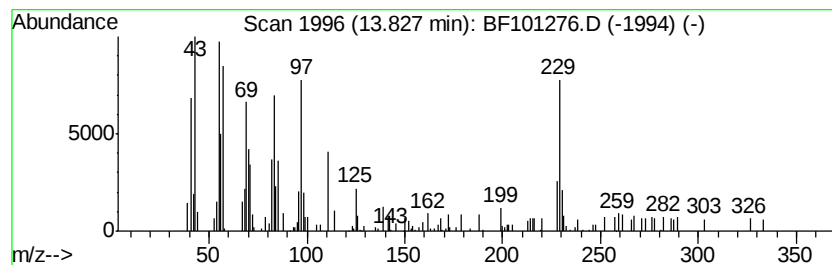
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	3.87 ng	71099	Chrysene-d12	14.01

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
2			1-Nonadecene	266	C19H38	018435-45-5	90
3			Cyclopentadecane	210	C15H30	000295-48-7	89
4			1-Tricosene	322	C23H46	018835-32-0	83
5			1-Eicosene	280	C20H40	003452-07-1	81



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Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PROS-1-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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...	5.05	4.2	ng	50525	1	6.83	240621	20.0
unknown6.60	6.60	76.6	ng	921447	1	6.83	240621	20.0
Tetradecane	9.79	2.1	ng	28935	3	9.87	274890	20.0
Hexadecane	10.29	2.1	ng	28260	3	9.87	274890	20.0
Naphtho[2,3-b]nor...	11.89	2.0	ng	28891	4	11.36	281478	20.0
4H-Cyclopenta[def...	11.98	3.5	ng	50026	4	11.36	281478	20.0
Pyrene, 1-methyl-	13.14	2.2	ng	41083	5	14.01	367619	20.0
Pentafluoropropio...	13.83	3.9	ng	71099	5	14.01	367619	20.0