

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102618\
 Data File : BF110213.D
 Acq On : 26 Oct 2018 16:50
 Operator : JU/SJ
 Sample : J5624-06
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PA-SB-03B

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-BF102318.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	2.310	33	38	50	rVB	338315	463658	15.47%	1.754%
2	3.599	256	257	267	rBV5	14815	36292	1.21%	0.137%
3	5.210	527	531	544	rVB	96297	120151	4.01%	0.455%
4	5.593	591	596	599	rBV	2714067	2519296	84.06%	9.531%
5	6.592	761	766	778	rBV2	2540607	2996977	100.00%	11.339%
6	6.740	786	791	794	rBV	2950133	2671019	89.12%	10.105%
7	6.969	826	830	833	rBV	871983	732546	24.44%	2.771%
8	7.122	852	856	860	rBV	2162858	2004445	66.88%	7.584%
9	7.528	920	925	934	rBV	1604730	1667802	55.65%	6.310%
10	8.251	1044	1048	1051	rBV	1063348	890821	29.72%	3.370%
11	9.328	1226	1231	1234	rBV	2739487	2611309	87.13%	9.880%
12	9.716	1293	1297	1304	rVB	388231	336624	11.23%	1.274%
13	10.010	1343	1347	1351	rBV	1092041	917444	30.61%	3.471%
14	10.416	1412	1416	1420	rVB4	29624	35353	1.18%	0.134%
15	10.804	1477	1482	1491	rBV	1438344	1443881	48.18%	5.463%
16	10.910	1495	1500	1503	rBV3	26420	41709	1.39%	0.158%
17	11.304	1565	1567	1572	rVB	33723	33755	1.13%	0.128%
18	11.398	1581	1583	1590	rVB	31949	31388	1.05%	0.119%
19	11.504	1597	1601	1603	rBV	932346	796776	26.59%	3.014%
20	11.527	1603	1605	1608	rVV	445927	341392	11.39%	1.292%
21	11.580	1611	1614	1617	rVV	63062	53693	1.79%	0.203%
22	11.733	1636	1640	1644	rVB2	38411	47520	1.59%	0.180%
23	12.010	1683	1687	1689	rBV2	144516	144326	4.82%	0.546%
24	12.033	1689	1691	1695	rVB2	75610	73408	2.45%	0.278%
25	12.116	1702	1705	1708	rBV2	47604	54674	1.82%	0.207%
26	12.298	1733	1736	1738	rBV2	43069	37047	1.24%	0.140%
27	12.327	1738	1741	1744	rBV2	55035	51560	1.72%	0.195%
28	12.721	1804	1808	1812	rBV	396860	361409	12.06%	1.367%
29	12.951	1841	1847	1853	rBV	372237	414049	13.82%	1.567%
30	13.086	1866	1870	1874	rBV	2138686	1837795	61.32%	6.953%
31	13.269	1899	1901	1905	rVB2	52082	55650	1.86%	0.211%
32	13.780	1986	1988	1993	rVB	38029	38874	1.30%	0.147%
33	13.968	2017	2020	2023	rBV2	176886	180514	6.02%	0.683%
34	14.151	2046	2051	2053	rBV2	769825	799227	26.67%	3.024%

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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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.174	2053	2055	2059	rVB	163809	138459	4.62%	0.524%
36	14.286	2072	2074	2078	rVB2	46394	43902	1.46%	0.166%
37	14.592	2124	2126	2132	rVB	73432	68472	2.28%	0.259%
38	14.915	2178	2181	2184	rVB	112551	117076	3.91%	0.443%
39	15.221	2230	2233	2237	rBV2	91500	138060	4.61%	0.522%
40	15.268	2239	2241	2246	rVB	132716	138482	4.62%	0.524%
41	15.610	2296	2299	2304	rVB	82475	110465	3.69%	0.418%
42	15.680	2306	2311	2323	rVB2	437919	675403	22.54%	2.555%
43	16.133	2385	2388	2396	rVB2	101754	158747	5.30%	0.601%

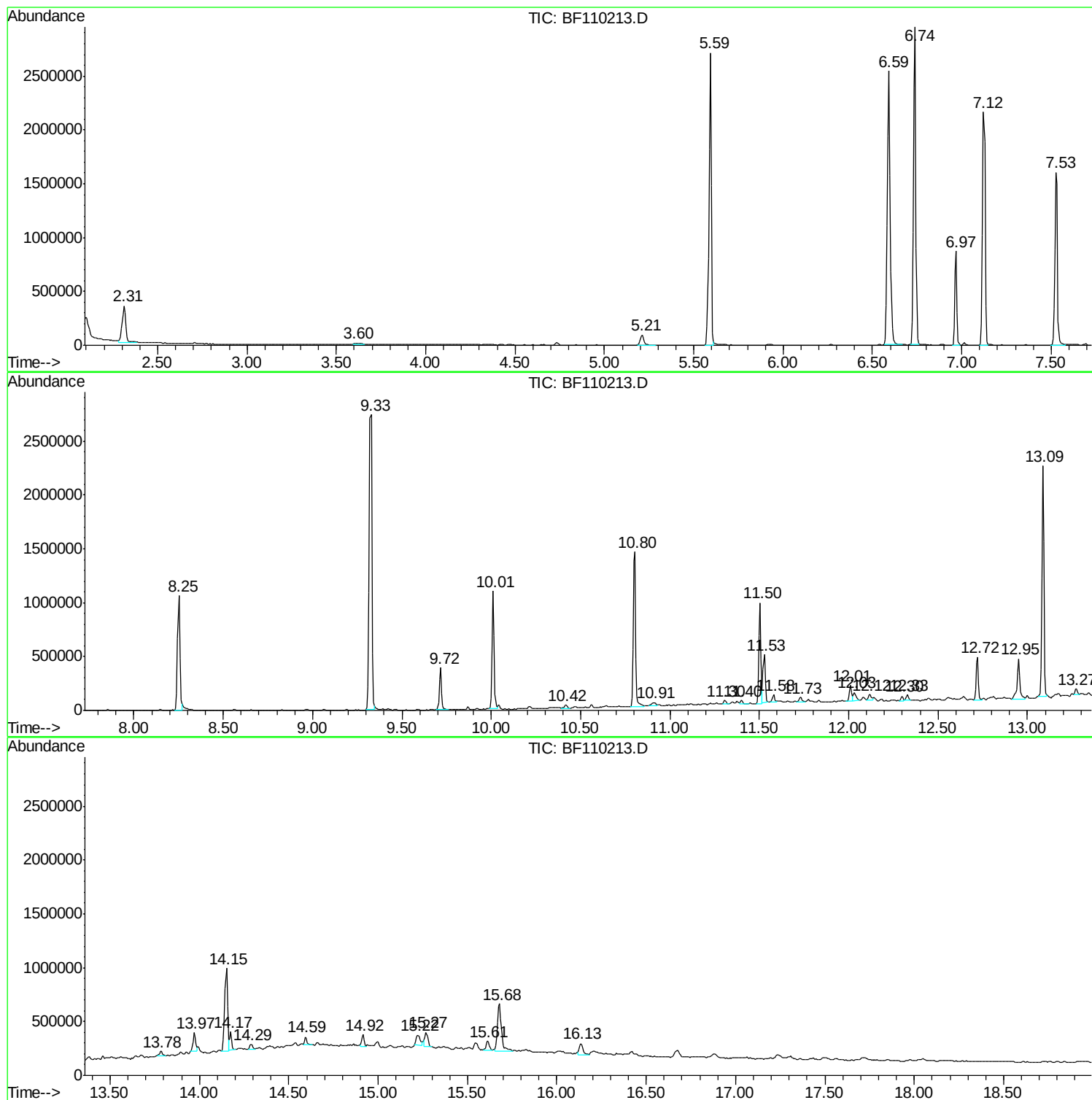
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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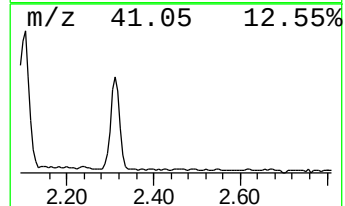
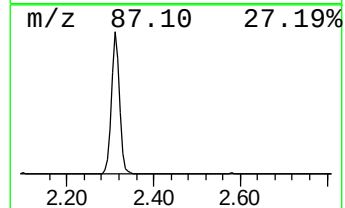
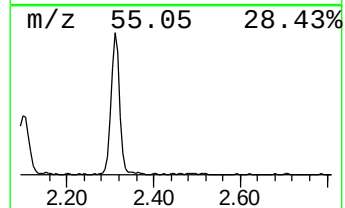
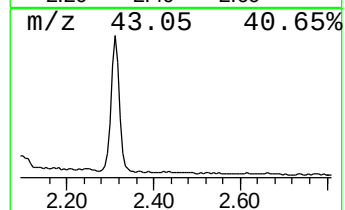
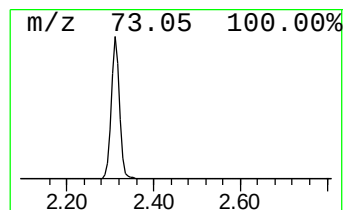
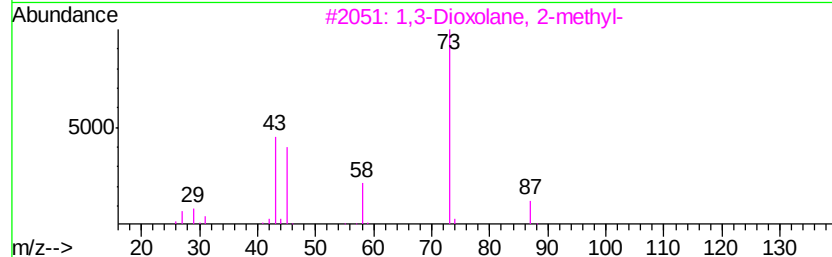
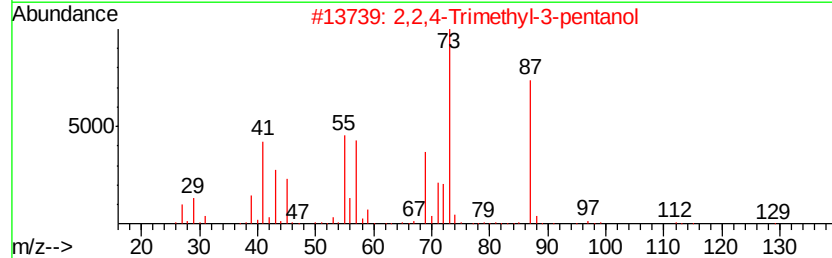
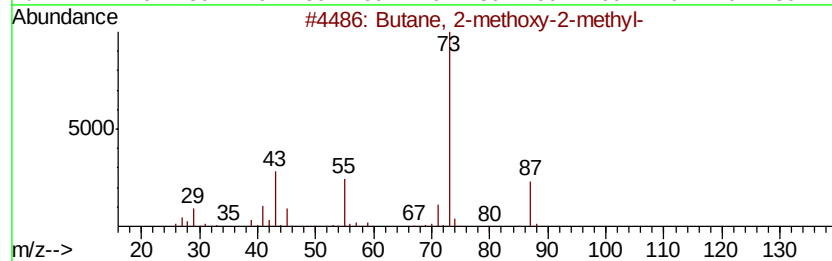
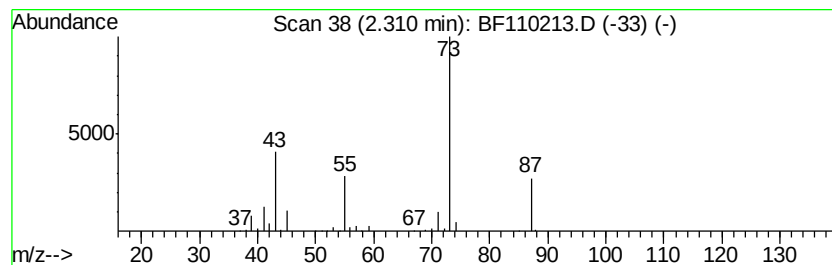
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.31	12.66 ng	463658	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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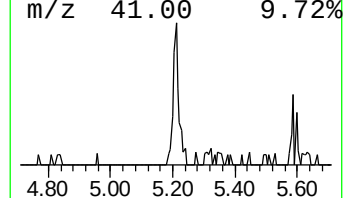
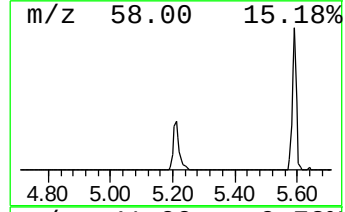
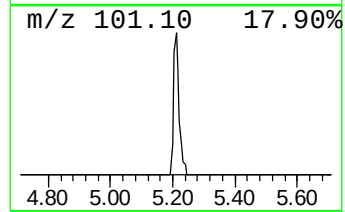
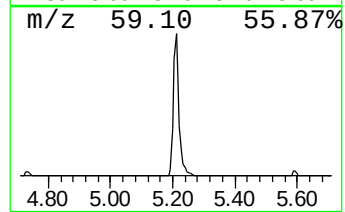
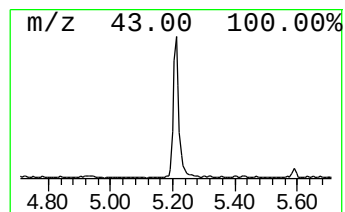
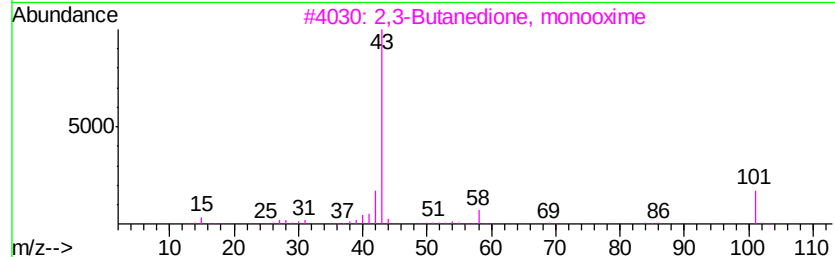
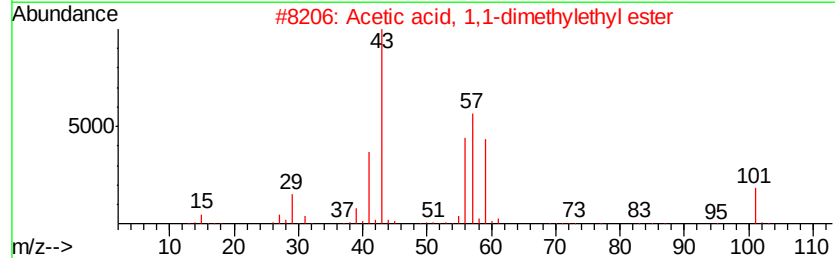
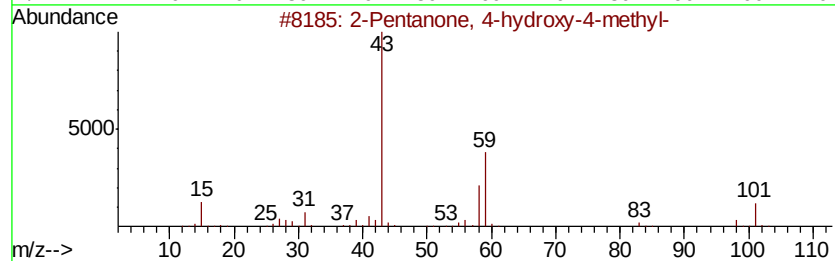
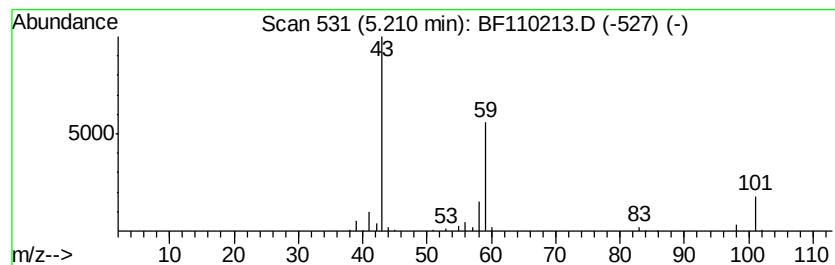
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	3.28 ng	120151	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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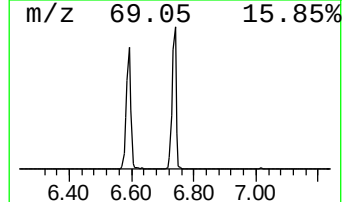
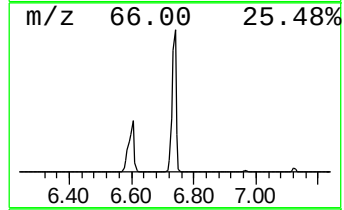
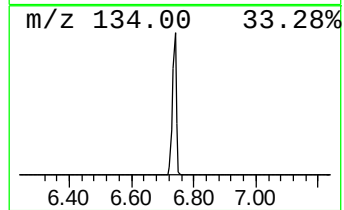
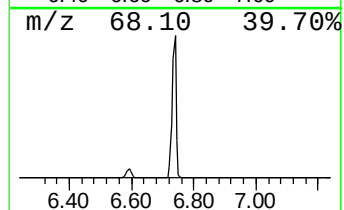
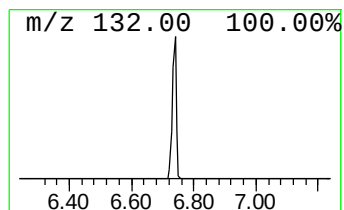
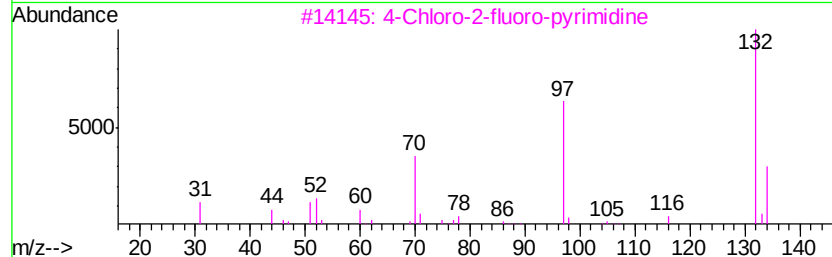
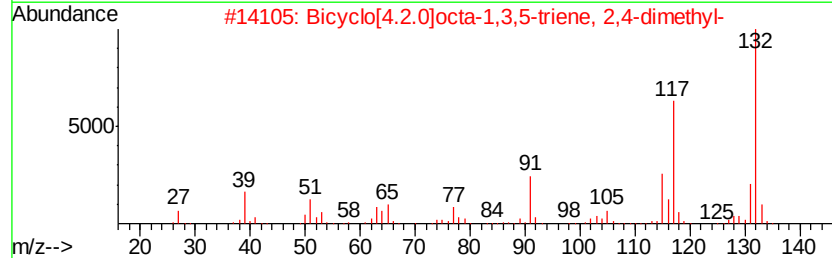
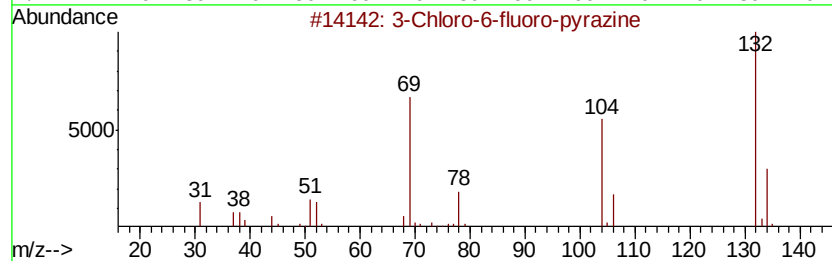
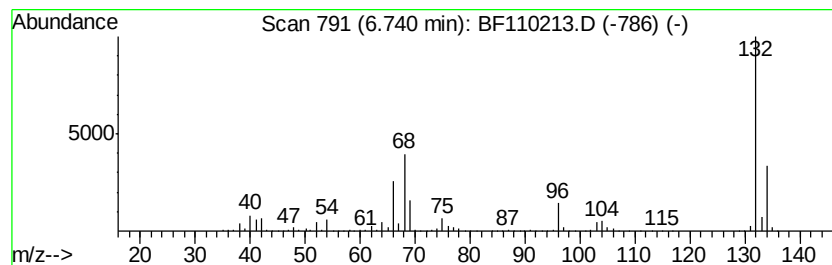
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF102318.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	72.92 ng	2671020	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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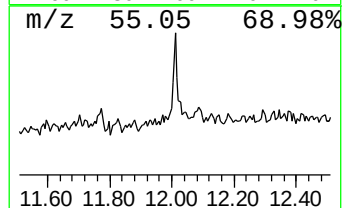
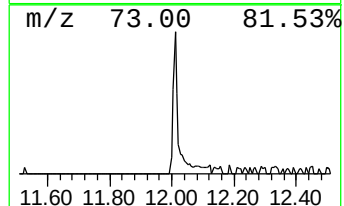
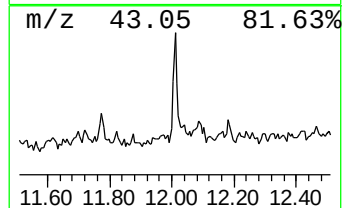
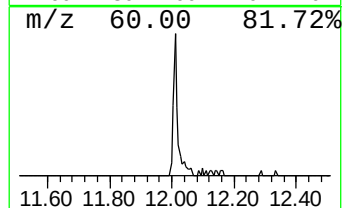
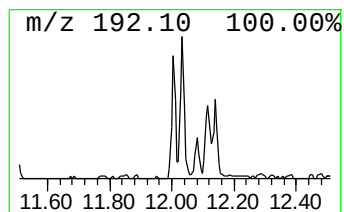
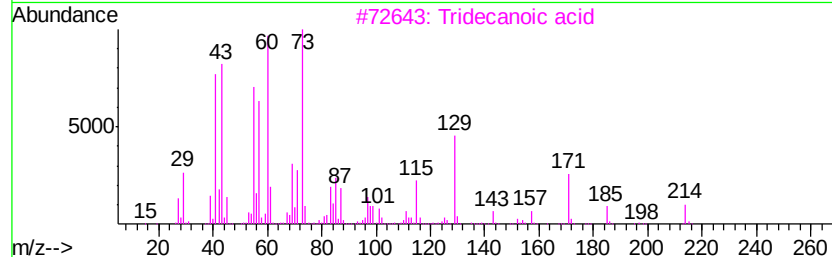
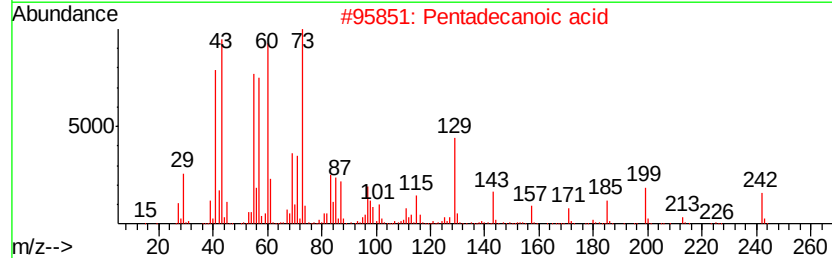
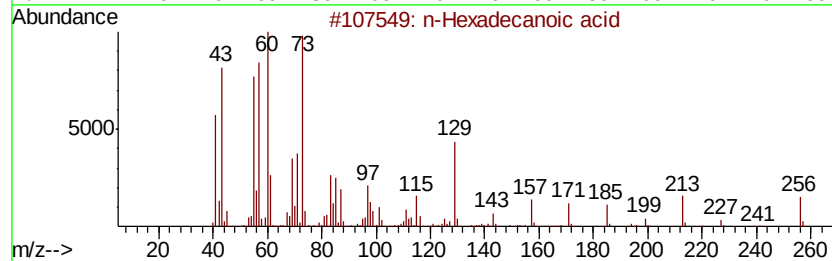
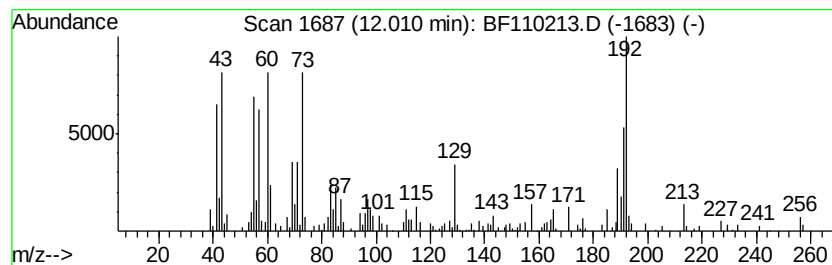
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	3.62 ng	144326	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	50
3	Tridecanoic acid	214	C13H26O2	000638-53-9	46
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	38
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	38



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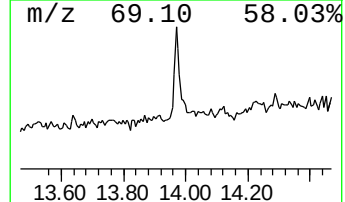
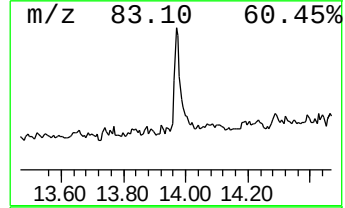
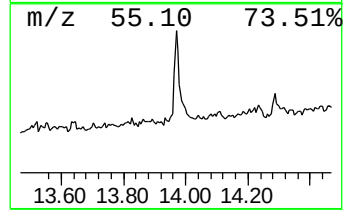
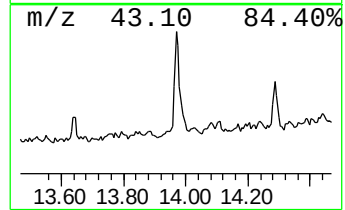
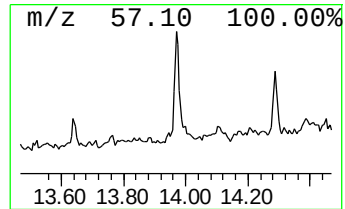
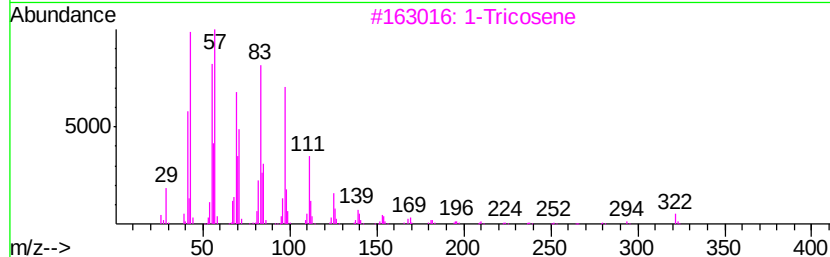
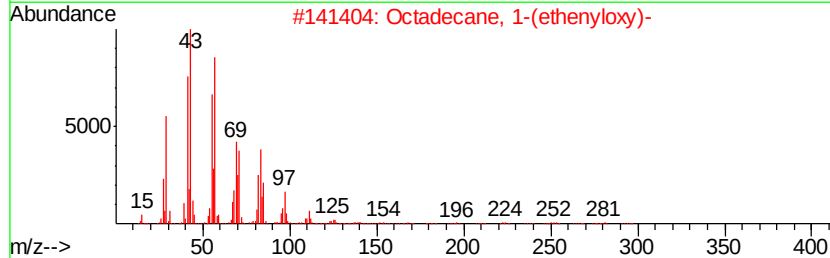
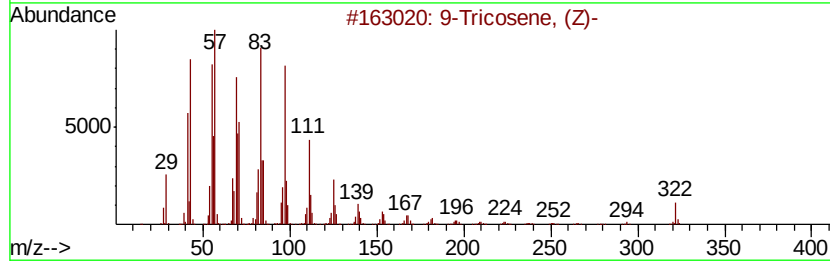
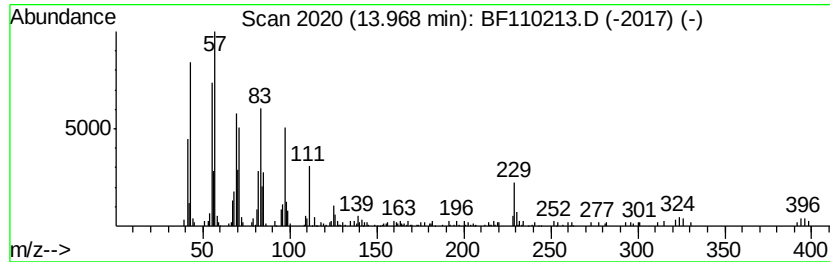
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 9-Tricosene, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	4.52 ng	180514	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Tricosene, (Z)-	322	C23H46	027519-02-4	98
2		Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	95
3		1-Tricosene	322	C23H46	018835-32-0	93
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	89
5		Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	87



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Data File : BF110213.D
Acq On : 26 Oct 2018 16:50
Operator : JU/SJ
Sample : J5624-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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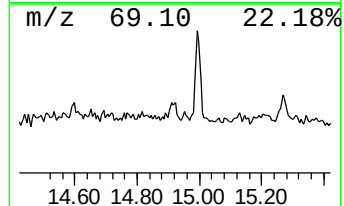
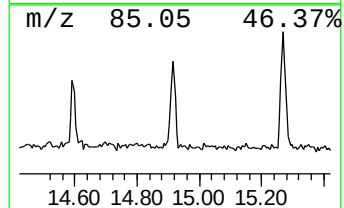
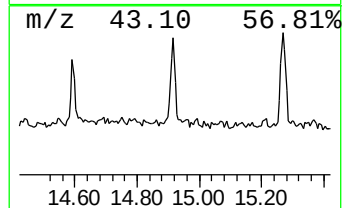
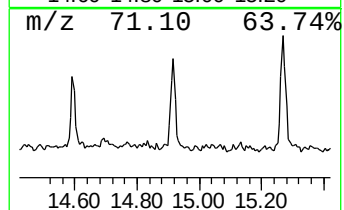
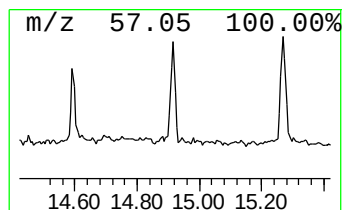
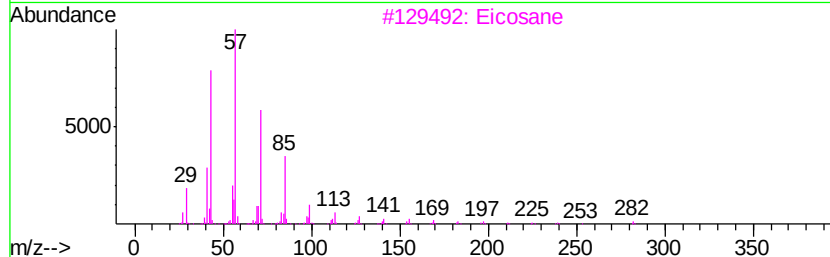
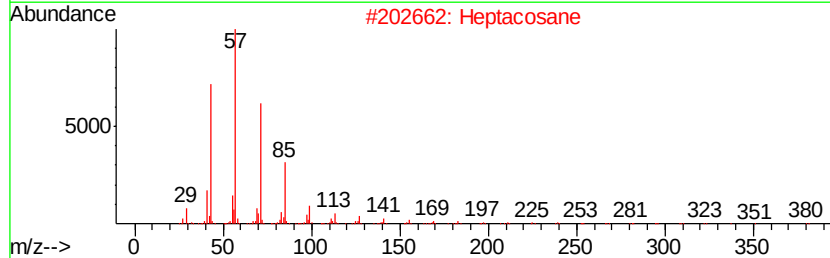
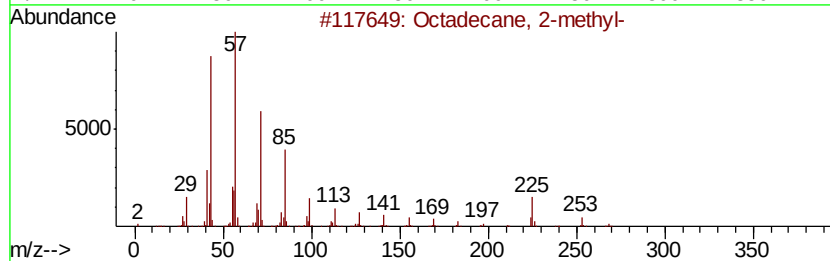
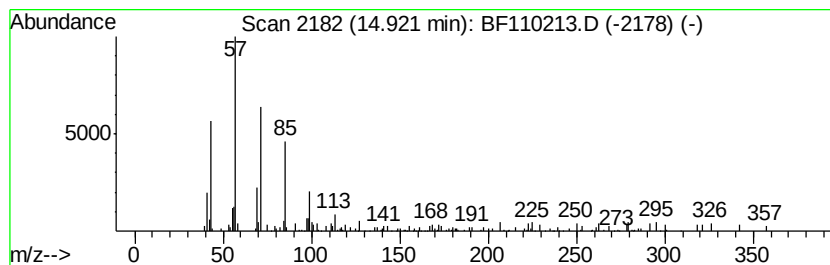
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	2.93 ng	117076	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
2		Heptacosane	380	C27H56	000593-49-7	87
3		Eicosane	282	C20H42	000112-95-8	80
4		Hentriacontane	437	C31H64	000630-04-6	78
5		Hexatriacontane	507	C36H74	000630-06-8	78



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102618\
Data File : BF110213.D
Acq On : 26 Oct 2018 16:50
Operator : JU/SJ
Sample : J5624-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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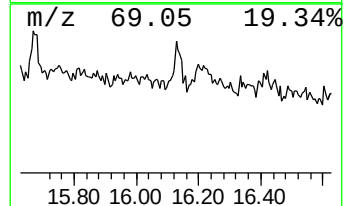
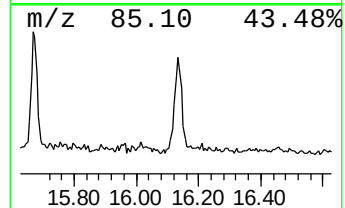
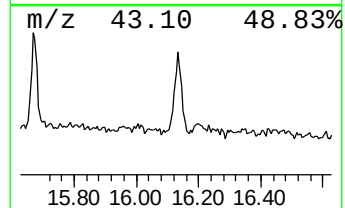
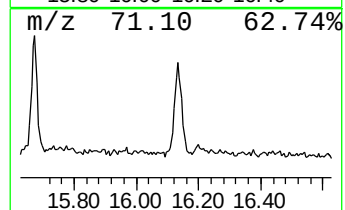
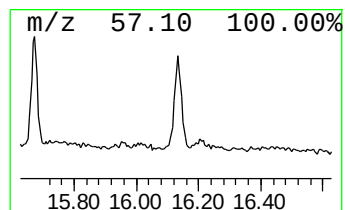
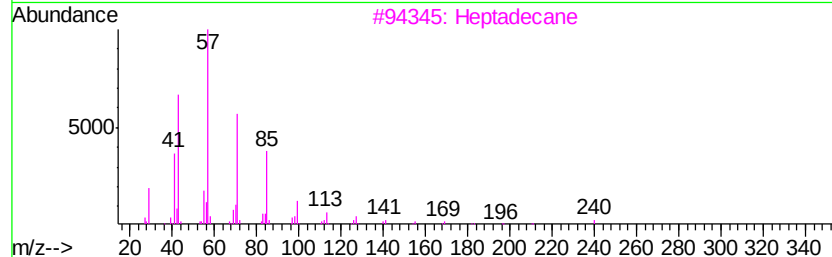
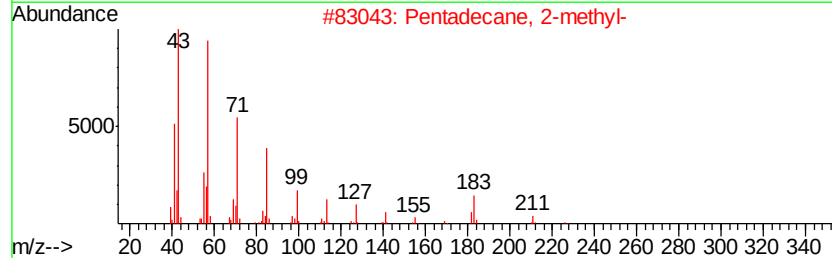
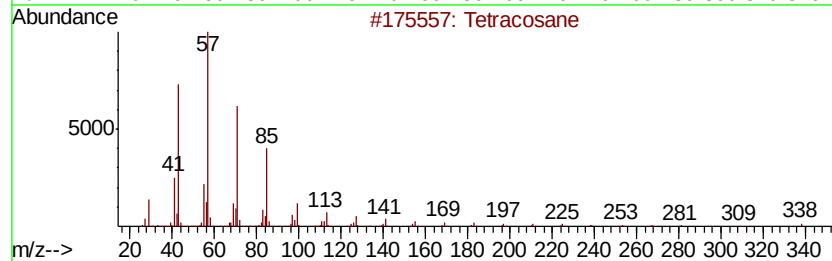
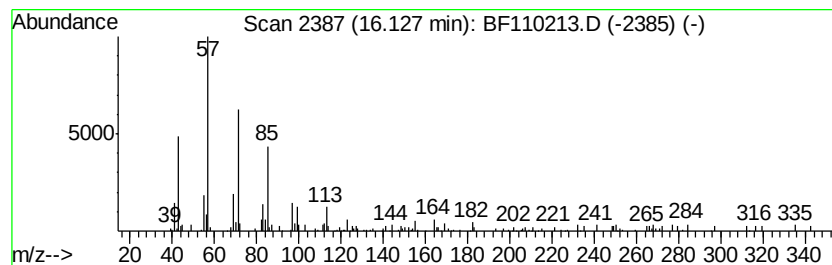
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	4.70 ng	158747	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	93
2		Pentadecane, 2-methyl-	226	C16H34	001560-93-6	87
3		Heptadecane	240	C17H36	000629-78-7	87
4		Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	86
5		Nonadecane	268	C19H40	000629-92-5	80



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Sample : J5624-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PA-SB-03B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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
Butane, 2-methoxy...	2.31	12.7	ng	463658	1	6.97	732546	20.0
2-Pentanone, 4-hy...	5.21	3.3	ng	120151	1	6.97	732546	20.0
unknown6.74	6.74	72.9	ng	2671020	1	6.97	732546	20.0
n-Hexadecanoic acid	12.01	3.6	ng	144326	4	11.50	796776	20.0
9-Tricosene, (Z)-	13.97	4.5	ng	180514	5	14.15	799227	20.0
Octadecane, 2-met...	14.92	2.9	ng	117076	5	14.15	799227	20.0
Tetracosane	16.13	4.7	ng	158747	6	15.68	675403	20.0