

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102518\
 Data File : BF110192.D
 Acq On : 26 Oct 2018 6:16
 Operator : JU/SJ
 Sample : J5658-02
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 JC-TS-002

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	368568	504634	14.85%	1.856%
2	5.210	528	531	538	rBV	97622	127436	3.75%	0.469%
3	5.592	591	596	599	rBV	2935716	2943457	86.59%	10.826%
4	6.592	760	766	781	rBV2	2803332	3399189	100.00%	12.502%
5	6.739	786	791	794	rBV	3302881	3042982	89.52%	11.192%
6	6.969	826	830	833	rBV	1029575	839756	24.70%	3.089%
7	7.122	852	856	860	rBV	2443304	2329778	68.54%	8.569%
8	7.534	920	926	929	rBV	1875478	1818864	53.51%	6.690%
9	8.251	1044	1048	1067	rVB	1179505	1038678	30.56%	3.820%
10	9.322	1226	1230	1234	rBV	2732795	2583938	76.02%	9.503%
11	9.639	1281	1284	1287	rBV	75395	56057	1.65%	0.206%
12	9.716	1293	1297	1304	rBV	391331	339116	9.98%	1.247%
13	10.010	1343	1347	1359	rVB2	1172558	991727	29.18%	3.647%
14	10.798	1477	1481	1492	rBV	1468584	1497431	44.05%	5.507%
15	11.504	1597	1601	1604	rBV	1003505	871809	25.65%	3.206%
16	12.716	1804	1807	1811	rBV	159472	148632	4.37%	0.547%
17	12.951	1840	1847	1852	rBV	152171	185624	5.46%	0.683%
18	13.086	1866	1870	1873	rBV	2033380	1711460	50.35%	6.295%
19	13.274	1895	1902	1904	rBV2	21267	35520	1.04%	0.131%
20	13.639	1960	1964	1967	rBV2	48126	51109	1.50%	0.188%
21	13.898	2002	2008	2011	rBV3	20023	38842	1.14%	0.143%
22	13.968	2015	2020	2030	rBV3	164432	256554	7.55%	0.944%
23	14.151	2046	2051	2053	rBV	799151	767535	22.58%	2.823%
24	14.174	2053	2055	2061	rVB	88977	78580	2.31%	0.289%
25	14.286	2071	2074	2080	rBV	61318	58635	1.72%	0.216%
26	14.592	2123	2126	2134	rVB	77775	84107	2.47%	0.309%
27	14.915	2177	2181	2185	rVB	87239	94126	2.77%	0.346%
28	15.221	2229	2233	2236	rBV	77431	114434	3.37%	0.421%
29	15.268	2238	2241	2245	rVB	114671	128974	3.79%	0.474%
30	15.545	2285	2288	2295	rVB	41090	59959	1.76%	0.221%
31	15.609	2295	2299	2304	rBV	56384	71265	2.10%	0.262%
32	15.674	2305	2310	2315	rBV2	469426	676640	19.91%	2.489%
33	16.133	2383	2388	2394	rVB	101319	153105	4.50%	0.563%
34	16.668	2475	2479	2487	rVB3	48994	89473	2.63%	0.329%

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Sample : J5658-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-TS-002

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

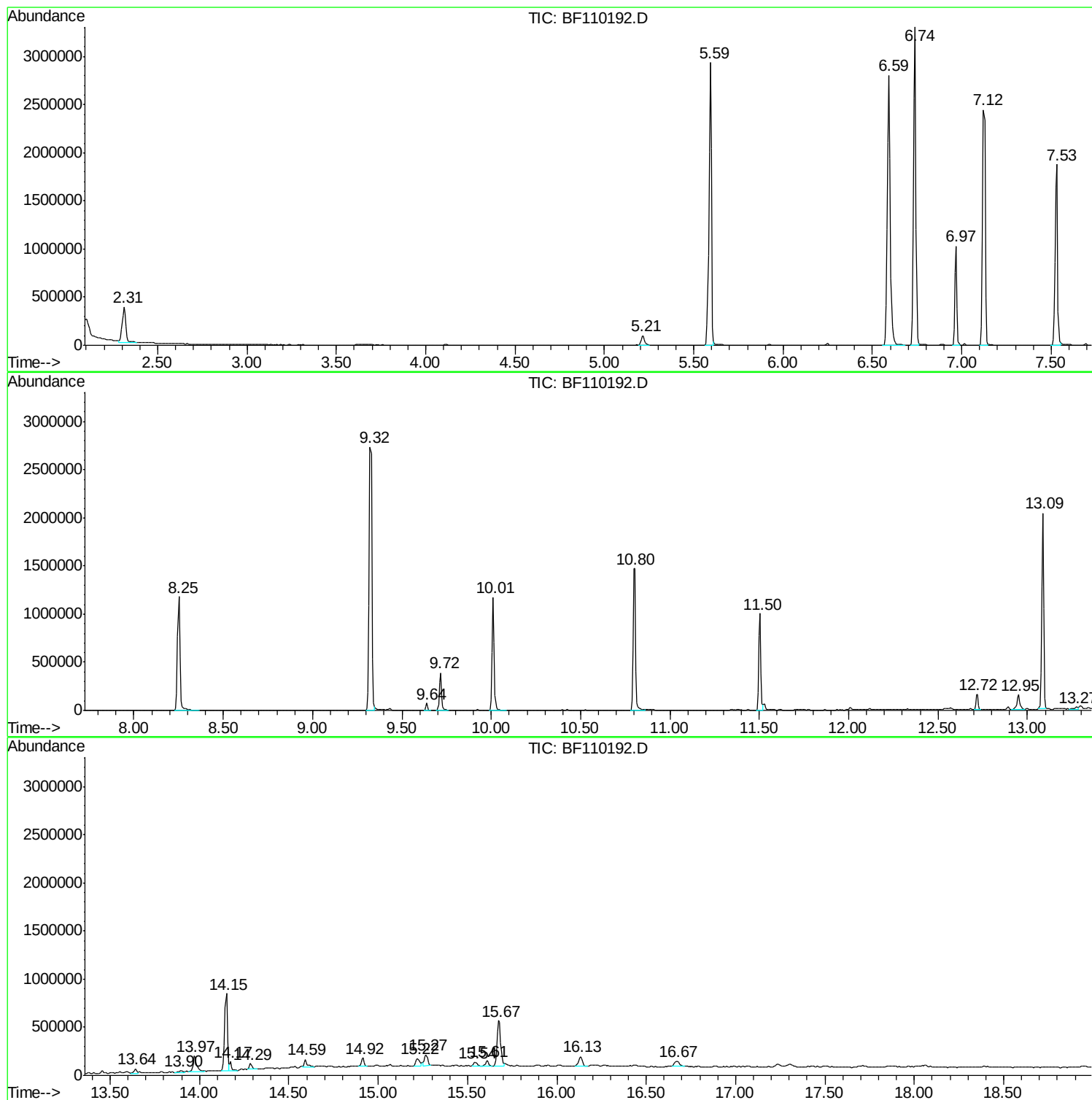
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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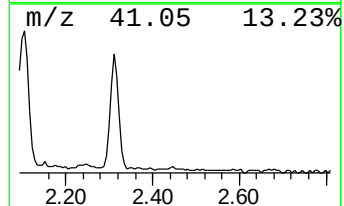
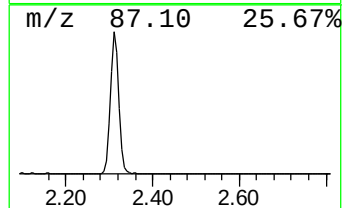
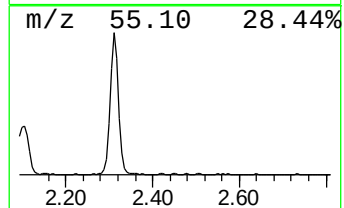
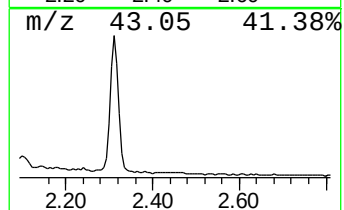
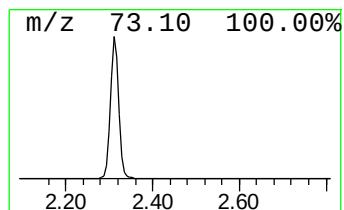
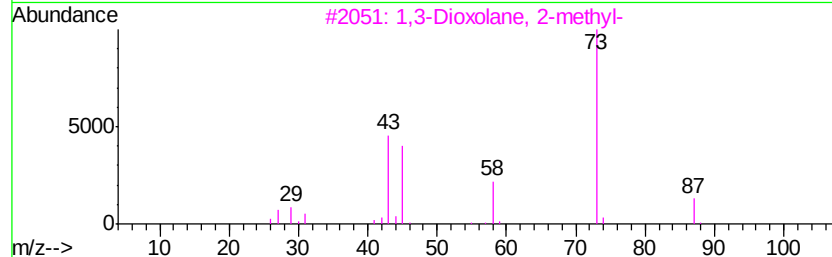
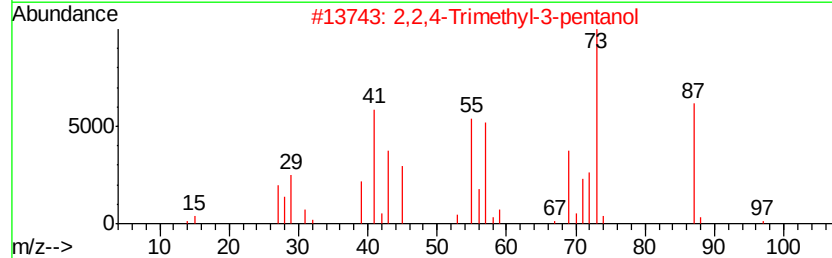
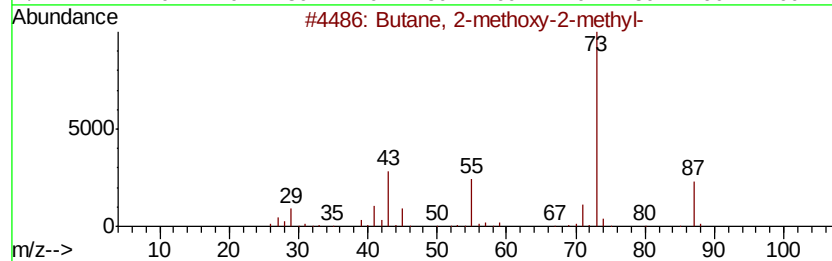
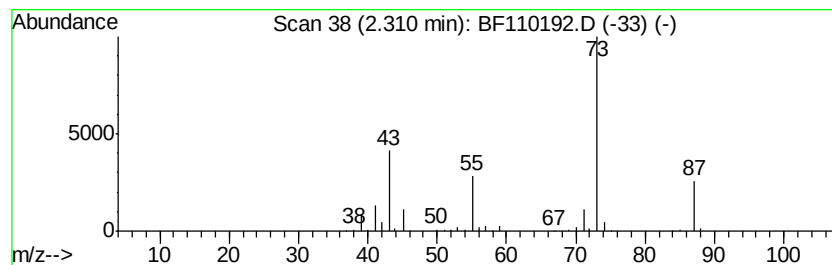
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.31	12.02 ng	504634	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	37
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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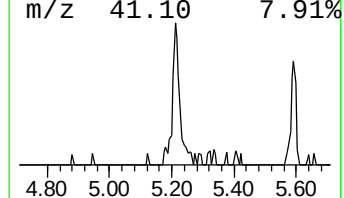
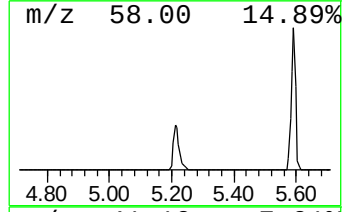
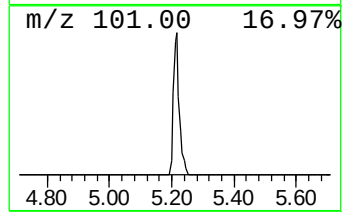
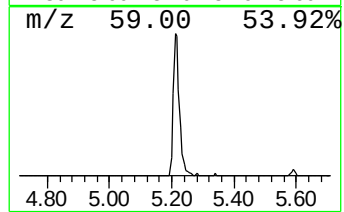
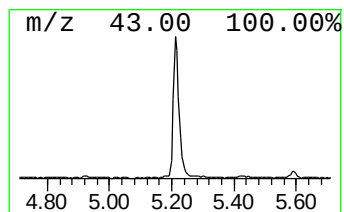
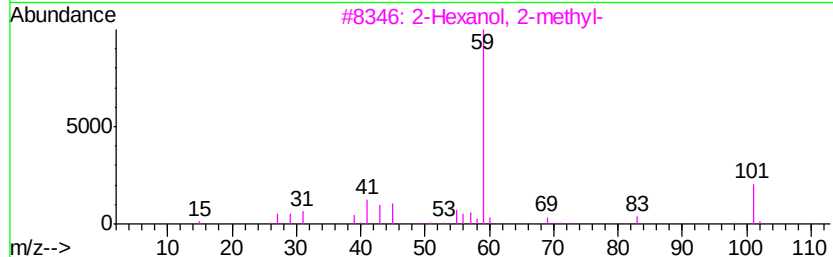
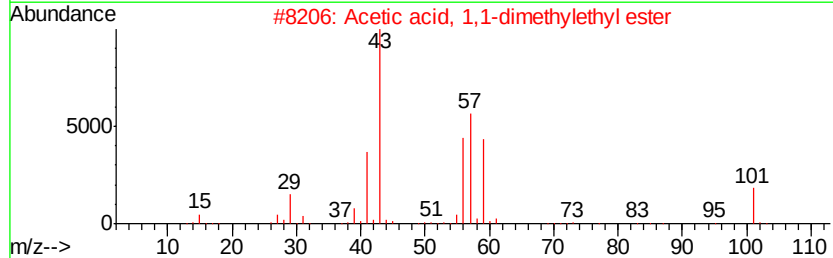
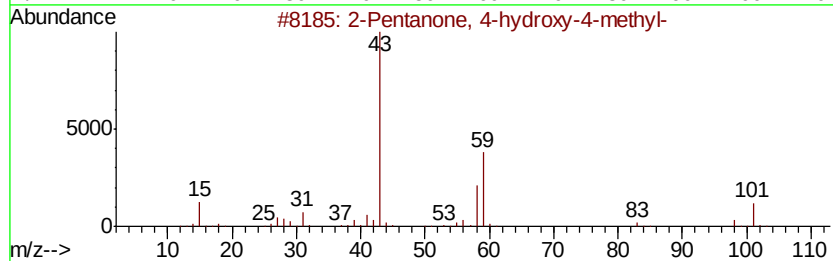
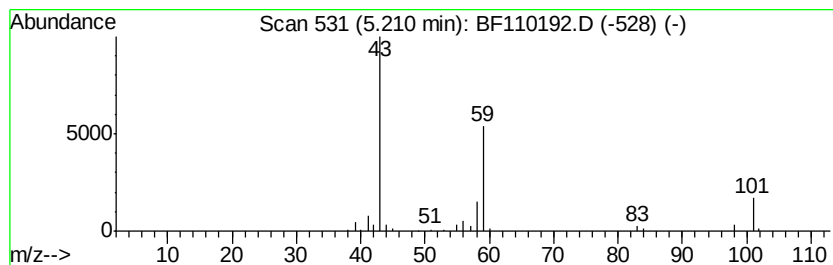
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	3.04 ng	127436	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	45
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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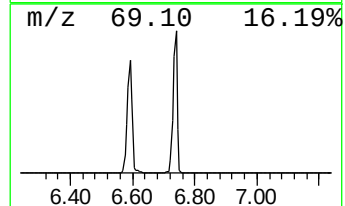
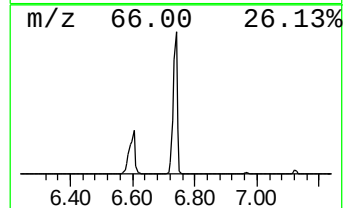
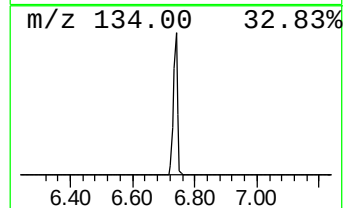
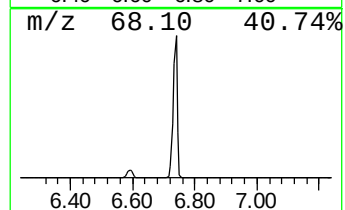
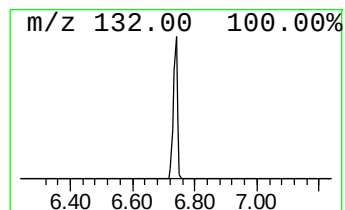
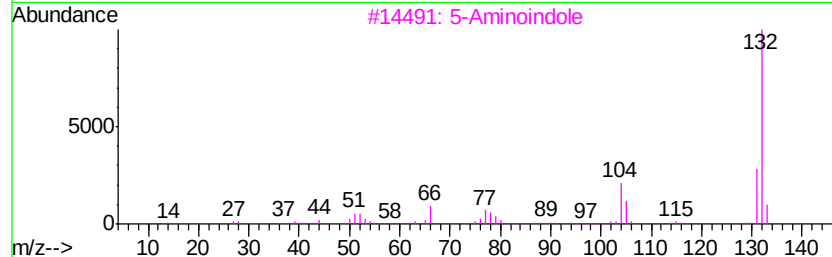
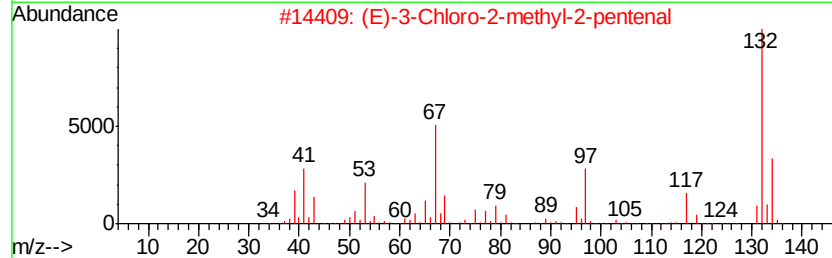
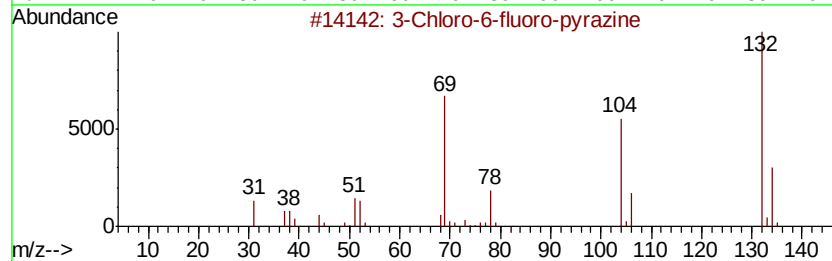
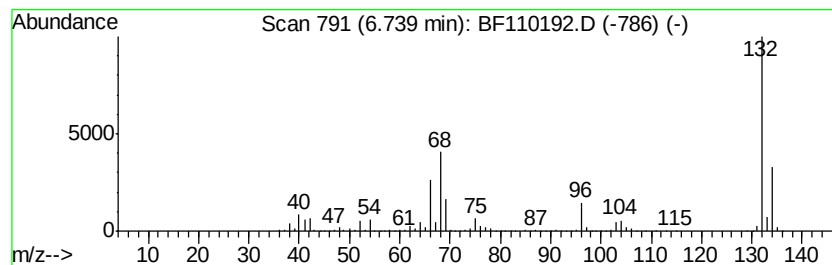
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	72.47 ng	3042980	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		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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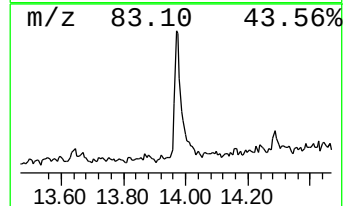
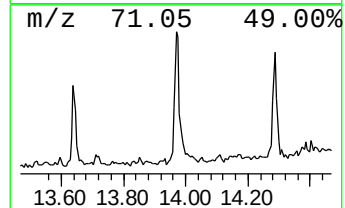
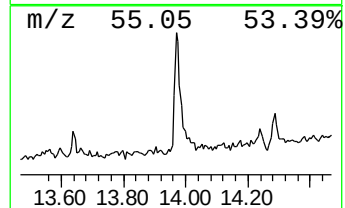
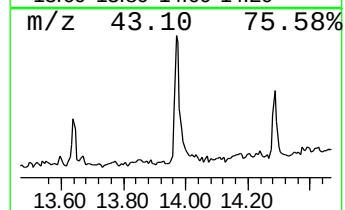
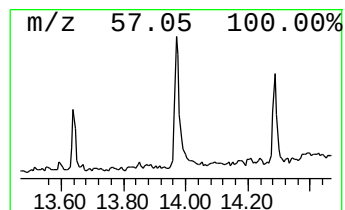
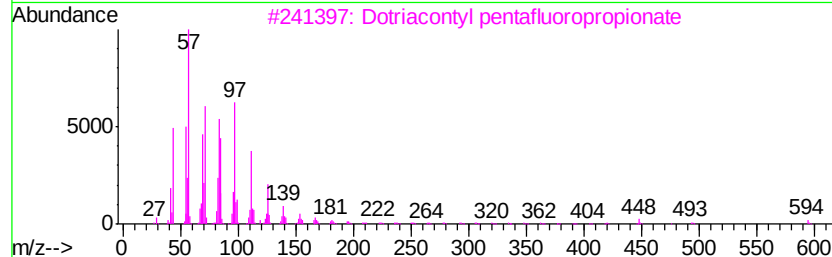
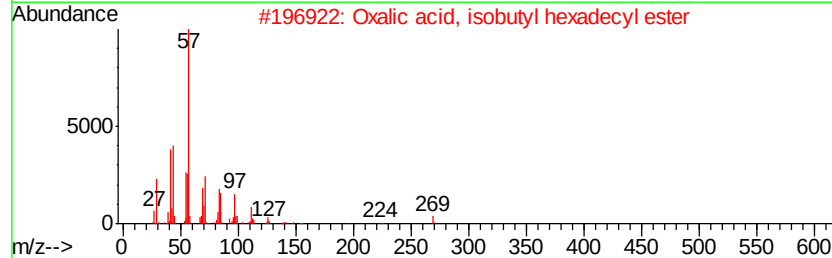
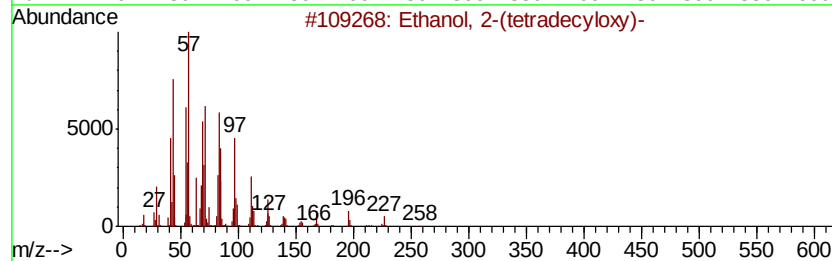
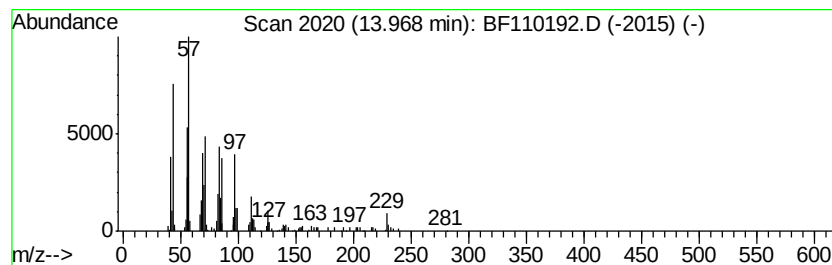
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Ethanol, 2-(tetradecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.97	6.69 ng	256554	Chrysene-d12	14.15		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2		Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
3		Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	91
4		Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	91
5		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	76



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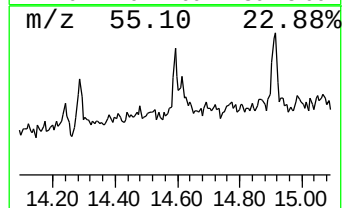
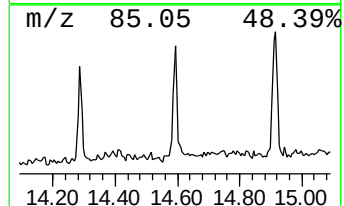
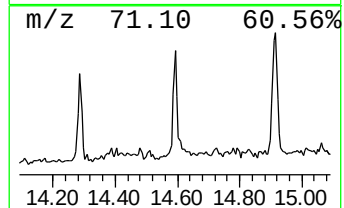
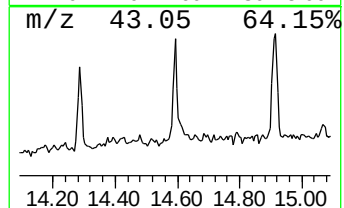
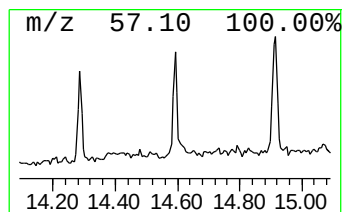
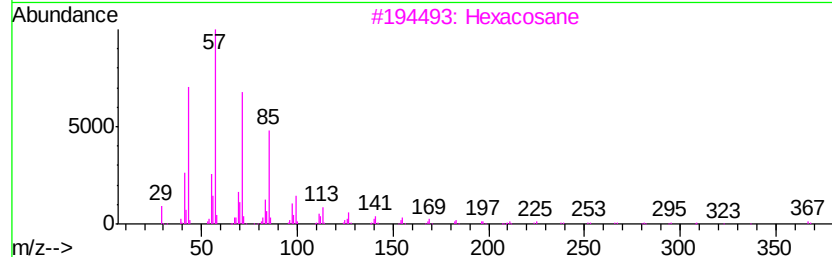
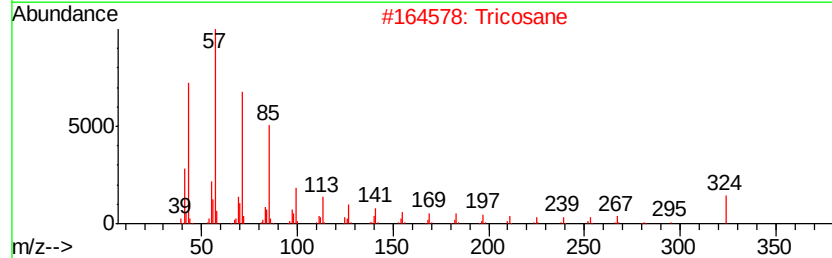
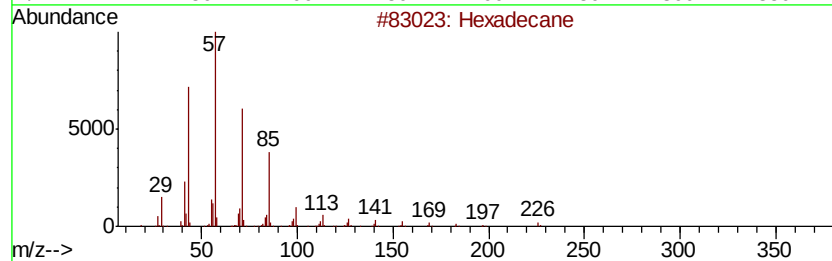
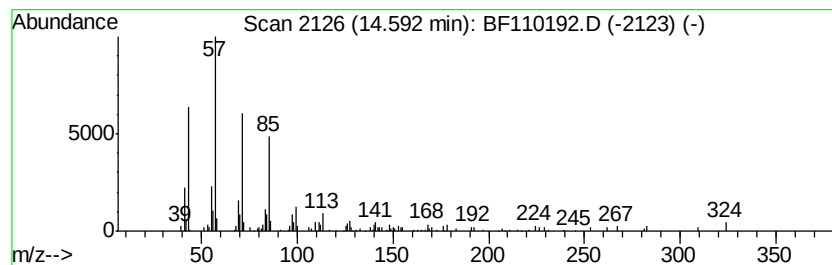
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.59	2.19 ng	84107	Chrysene-d12		14.15
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	96
2	Tricosane	324	C23H48	000638-67-5	90
3	Hexacosane	366	C26H54	000630-01-3	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Octacosane	394	C28H58	000630-02-4	83



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 ClientSampleId :
 JC-TS-002

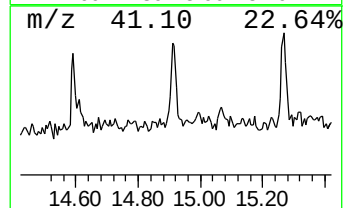
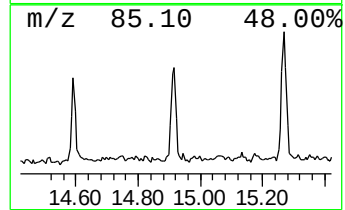
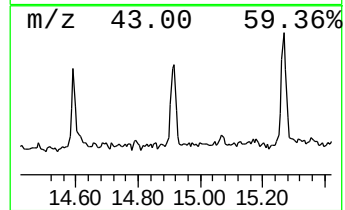
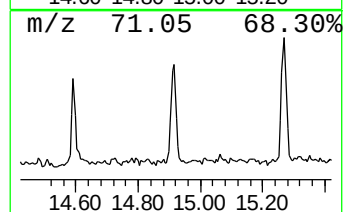
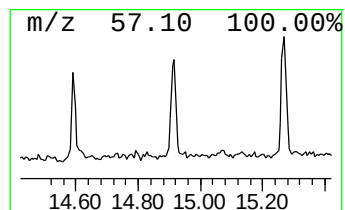
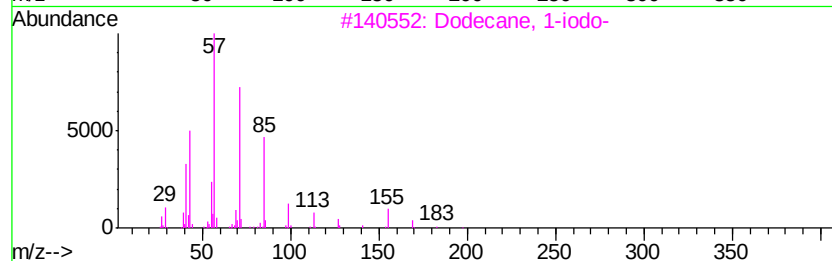
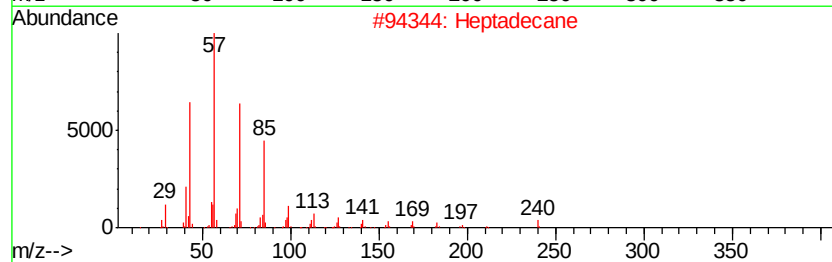
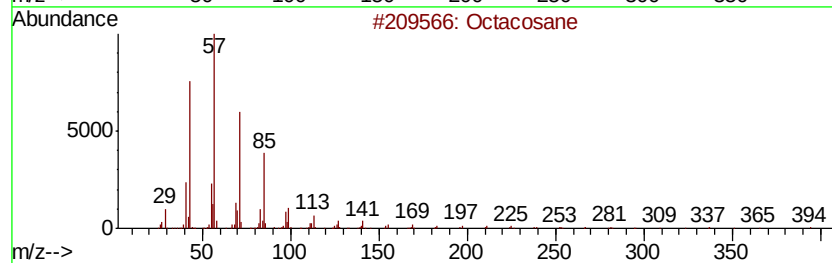
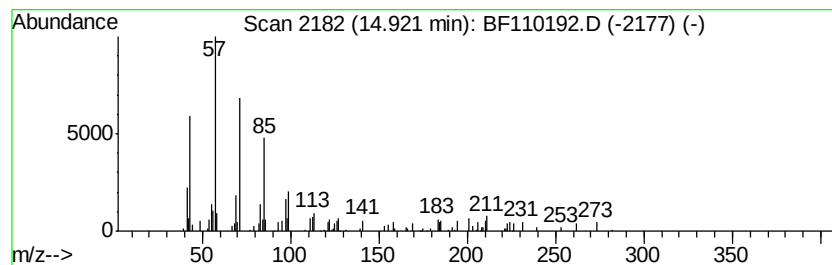
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	2.78 ng	94126	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	87
2		Heptadecane	240	C17H36	000629-78-7	83
3		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	83
4		Heneicosane	296	C21H44	000629-94-7	81
5		2-methyloctacosane	408	C29H60	1000376-72-8	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102518\
Data File : BF110192.D
Acq On : 26 Oct 2018 6:16
Operator : JU/SJ
Sample : J5658-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-TS-002

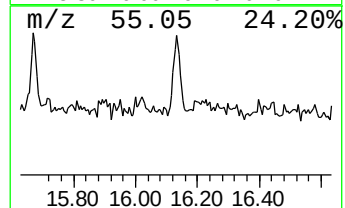
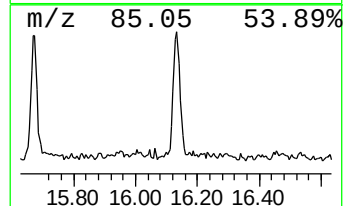
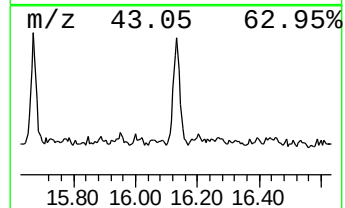
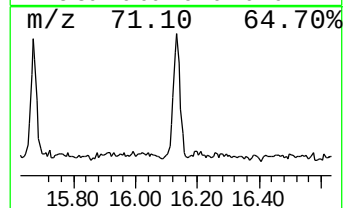
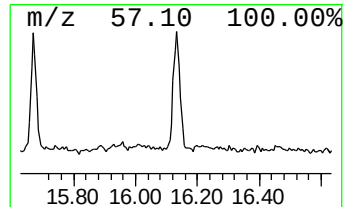
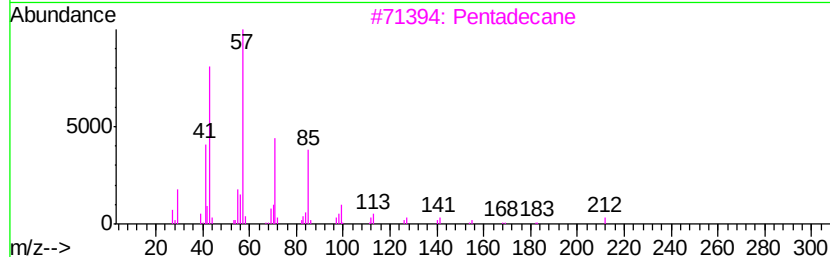
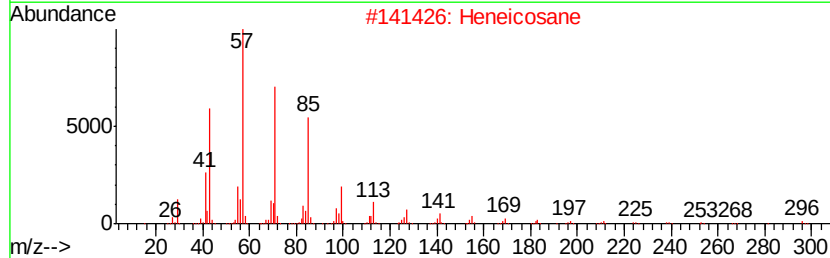
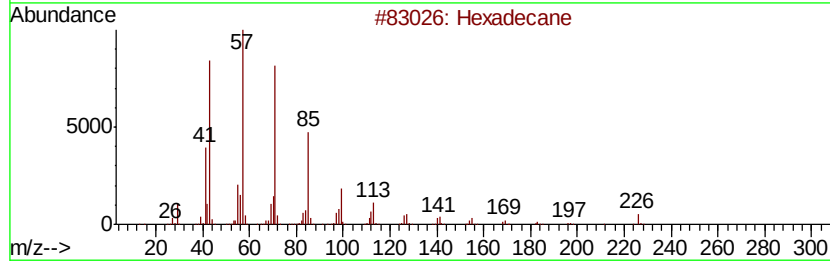
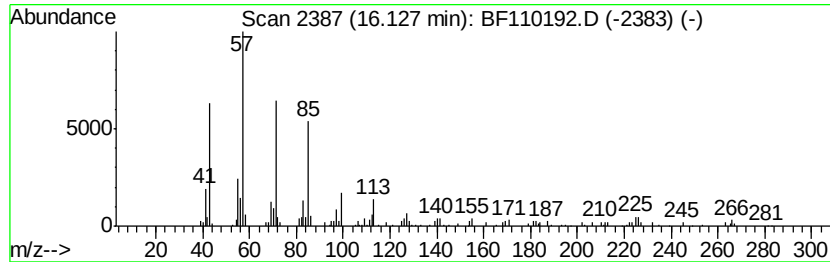
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	4.53 ng	153105	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	90
2		Heneicosane	296	C21H44	000629-94-7	87
3		Pentadecane	212	C15H32	000629-62-9	87
4		Heptadecane	240	C17H36	000629-78-7	86
5		Tridecane, 3-methyl-	198	C14H30	006418-41-3	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102518\
Data File : BF110192.D
Acq On : 26 Oct 2018 6:16
Operator : JU/SJ
Sample : J5658-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-TS-002

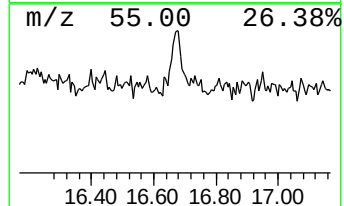
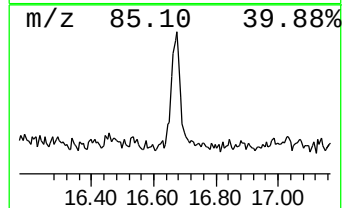
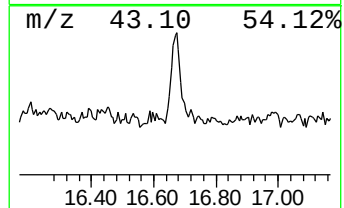
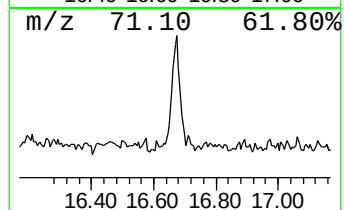
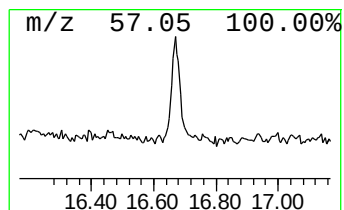
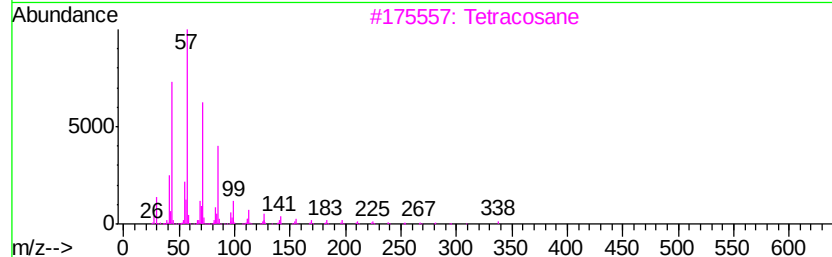
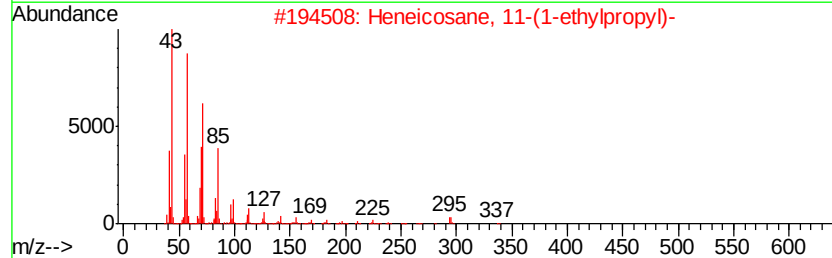
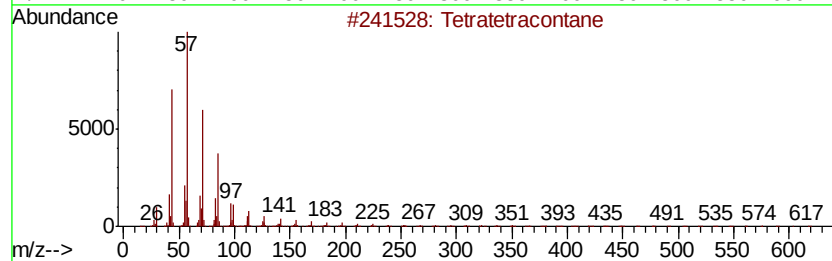
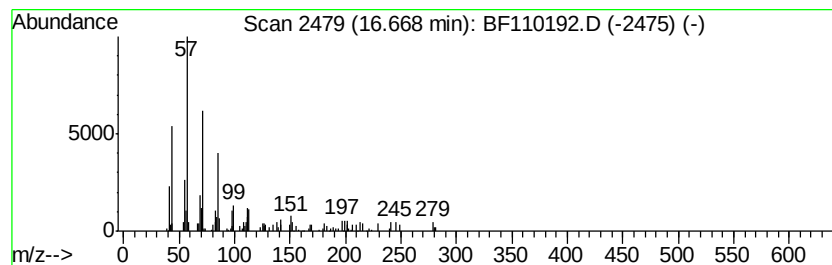
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetratetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.67	2.64 ng	89473	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	83
2		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	80
3		Tetracosane	338	C24H50	000646-31-1	72
4		Octacosane	394	C28H58	000630-02-4	72
5		2-methyloctacosane	408	C29H60	1000376-72-8	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102518\
Data File : BF110192.D
Acq On : 26 Oct 2018 6:16
Operator : JU/SJ
Sample : J5658-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-TS-002

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
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2-Pentanone, 4-hy...	5.21	3.0	ng	127436	1	6.97	839756	20.0
unknown6.74	6.74	72.5	ng	3042980	1	6.97	839756	20.0
Ethanol, 2-(tetra...	13.97	6.7	ng	256554	5	14.15	767535	20.0
Hexadecane	14.59	2.2	ng	84107	5	14.15	767535	20.0
Octacosane	14.92	2.8	ng	94126	6	15.68	676640	20.0
Heneicosane	16.13	4.5	ng	153105	6	15.68	676640	20.0
Tetratetracontane	16.67	2.6	ng	89473	6	15.68	676640	20.0