

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100518\
 Data File : BF109626.D
 Acq On : 5 Oct 2018 23:24
 Operator : JU/SJ
 Sample : J5263-07
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GRID16-COMP-100318

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-BF092218.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	4.893	474	477	486	rVB	38630	47463	3.24%	0.330%
2	5.322	546	550	580	rBV	1095396	1228705	83.92%	8.541%
3	6.351	721	725	742	rBV	1210004	1412098	96.45%	9.816%
4	6.475	742	746	762	rVB	1413369	1390284	94.96%	9.664%
5	6.698	781	784	795	rBV	399773	463026	31.63%	3.219%
6	6.857	807	811	827	rBV	1180650	1069328	73.04%	7.433%
7	7.263	876	880	909	rBV	811629	920856	62.90%	6.401%
8	7.981	998	1002	1023	rBV	598282	618234	42.23%	4.297%
9	9.057	1181	1185	1201	rBV	1532411	1464086	100.00%	10.177%
10	9.451	1248	1252	1260	rBV	139269	133904	9.15%	0.931%
11	9.728	1295	1299	1317	rBV	646594	636479	43.47%	4.424%
12	10.516	1429	1433	1452	rBV	683529	753163	51.44%	5.235%
13	11.210	1547	1551	1554	rBV	516548	533296	36.43%	3.707%
14	11.745	1639	1642	1648	rBV2	47791	56210	3.84%	0.391%
15	12.416	1752	1756	1761	rBV	68554	70189	4.79%	0.488%
16	12.639	1788	1794	1798	rBV2	59344	67489	4.61%	0.469%
17	12.786	1815	1819	1828	rVB	1266426	1105066	75.48%	7.681%
18	13.027	1854	1860	1864	rBV2	23495	25741	1.76%	0.179%
19	13.269	1894	1901	1908	rBV7	5995	14706	1.00%	0.102%
20	13.369	1912	1918	1920	rBV2	34156	32309	2.21%	0.225%
21	13.692	1968	1973	1982	rBV2	103167	149955	10.24%	1.042%
22	13.833	1992	1997	2007	rBV	600921	616229	42.09%	4.283%
23	14.010	2024	2027	2030	rBV	62574	56566	3.86%	0.393%
24	14.310	2075	2078	2082	rBV	90057	84802	5.79%	0.589%
25	14.604	2125	2128	2134	rBV	124913	114944	7.85%	0.799%
26	14.674	2136	2140	2146	rVV	72115	67572	4.62%	0.470%
27	14.845	2164	2169	2171	rBV	31298	45738	3.12%	0.318%
28	14.916	2177	2181	2190	rBV	136444	156425	10.68%	1.087%
29	15.121	2212	2216	2221	rBV2	17715	26392	1.80%	0.183%
30	15.174	2222	2225	2230	rVB	27062	36401	2.49%	0.253%
31	15.233	2230	2235	2238	rBV	403848	494125	33.75%	3.435%
32	15.268	2238	2241	2249	rVB	144145	178206	12.17%	1.239%
33	15.663	2304	2308	2313	rBV	104113	141739	9.68%	0.985%
34	16.127	2381	2387	2398	rVB2	68595	127259	8.69%	0.885%

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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-BF092218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.657	2473	2477	2484	rVB3	26324	47273	3.23%	0.329%
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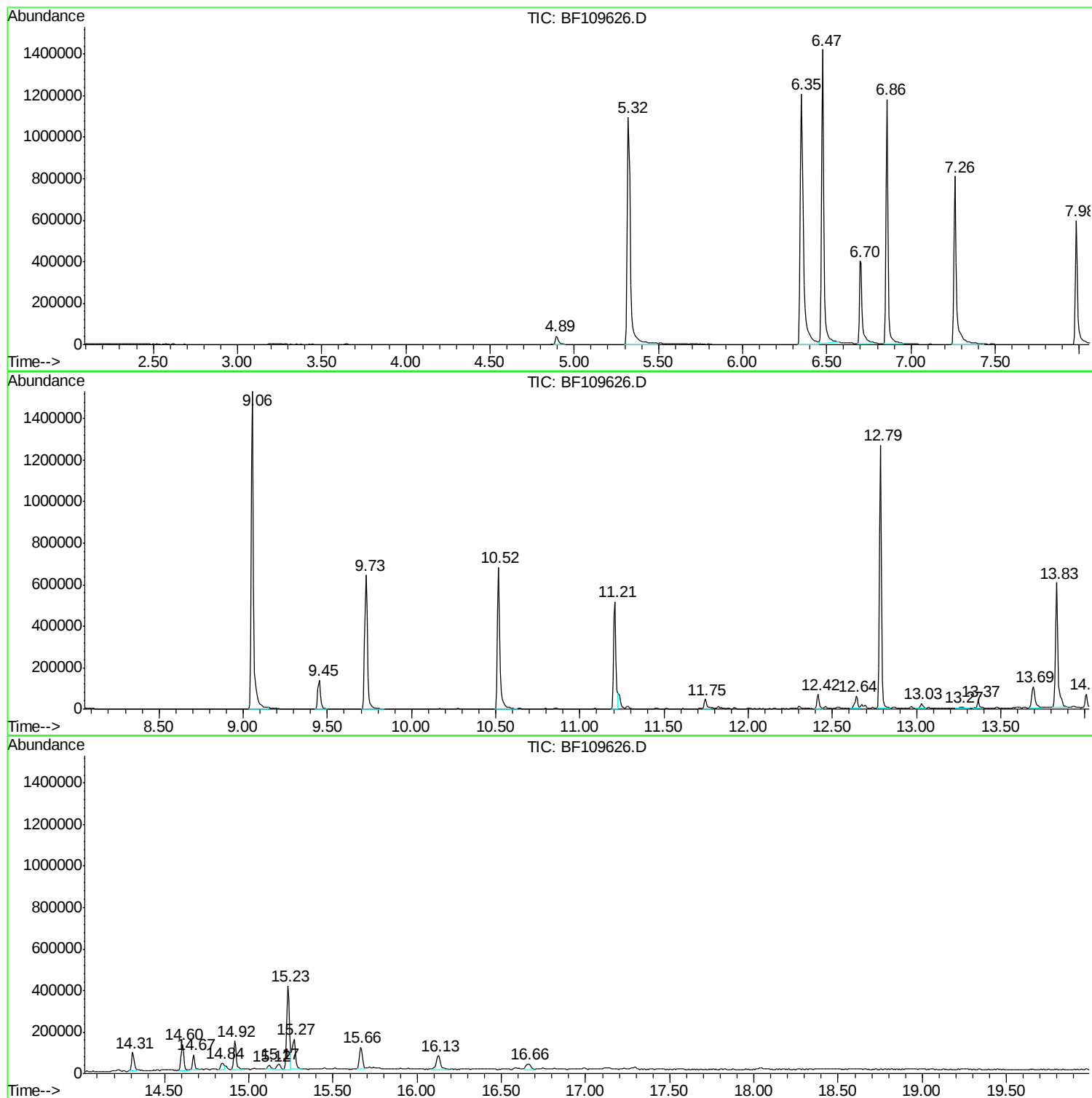
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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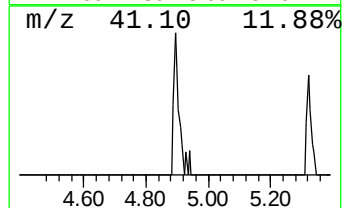
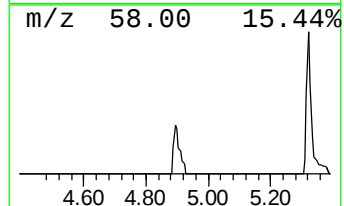
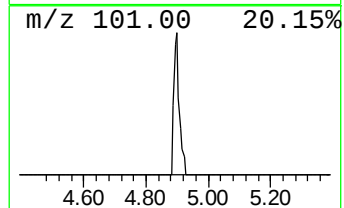
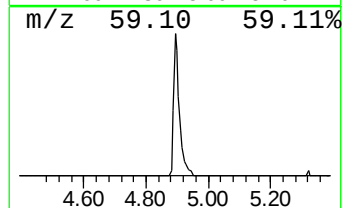
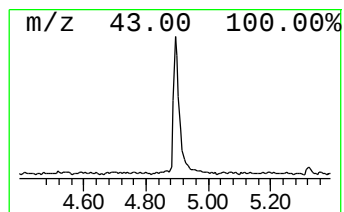
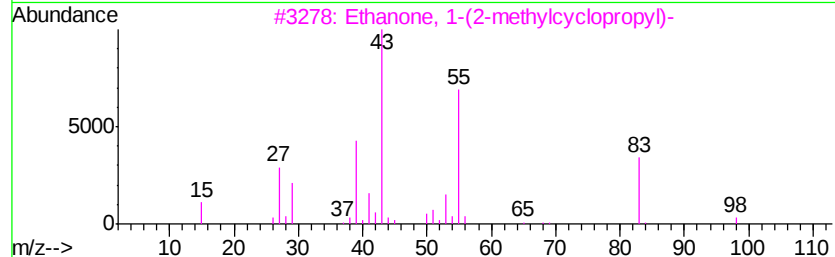
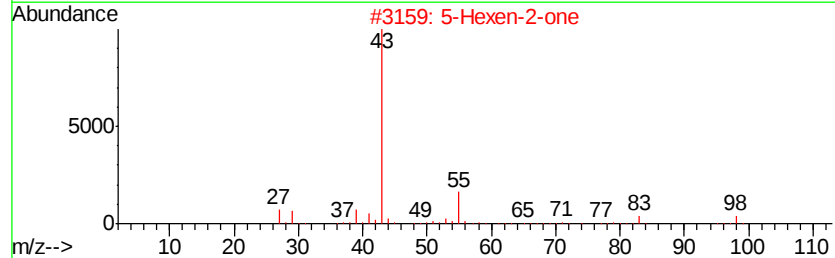
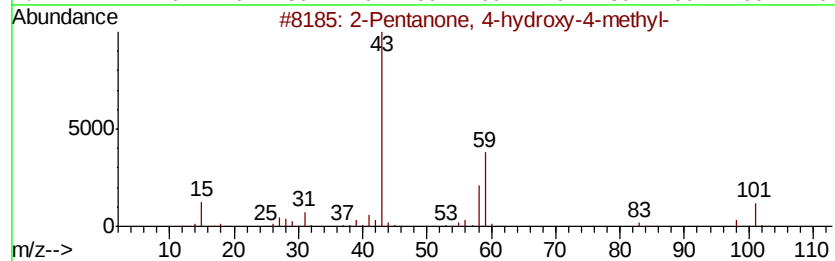
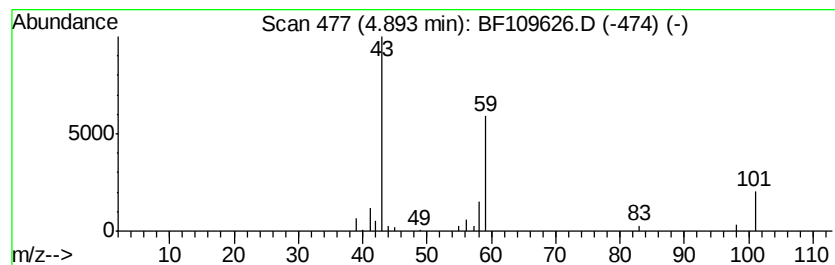
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	2.05 ng	47463	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			5-Hexen-2-one	98	C6H10O	000109-49-9	9
3			Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
4			3-Octanol	130	C8H18O	000589-98-0	9
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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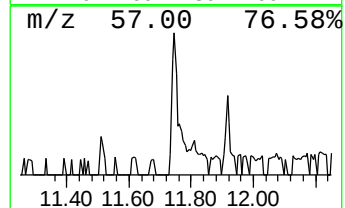
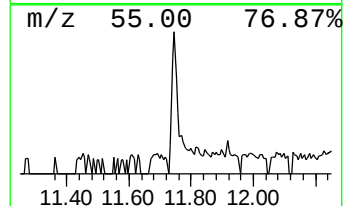
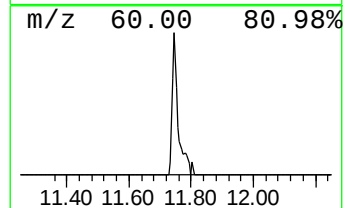
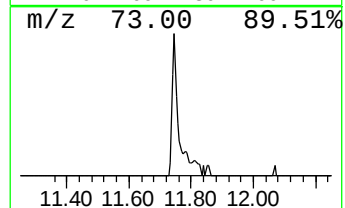
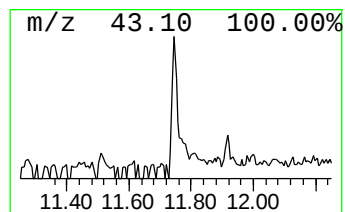
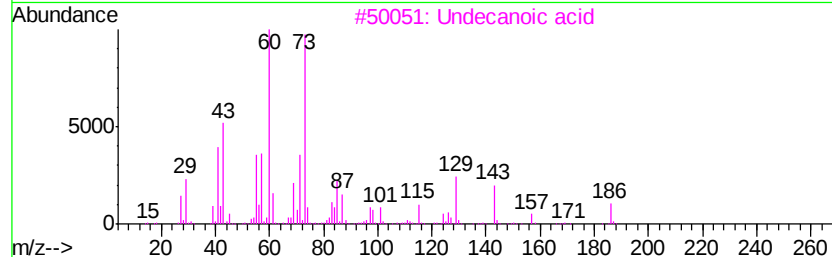
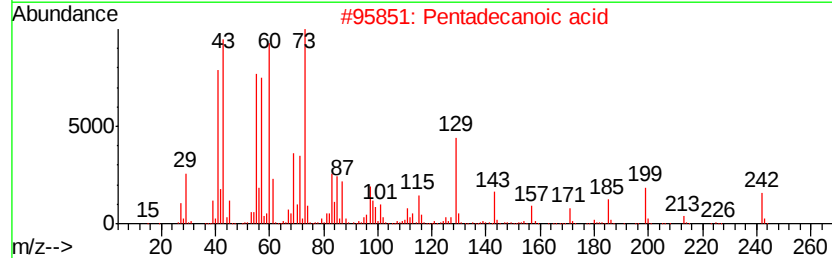
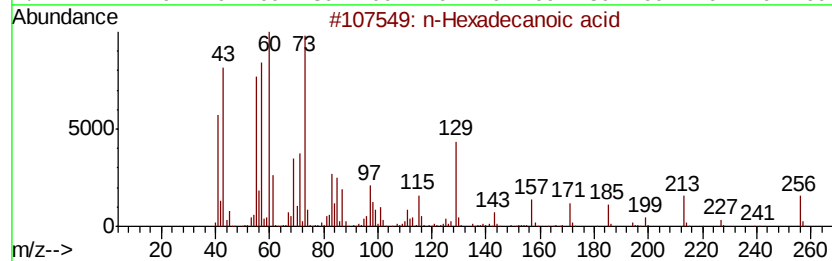
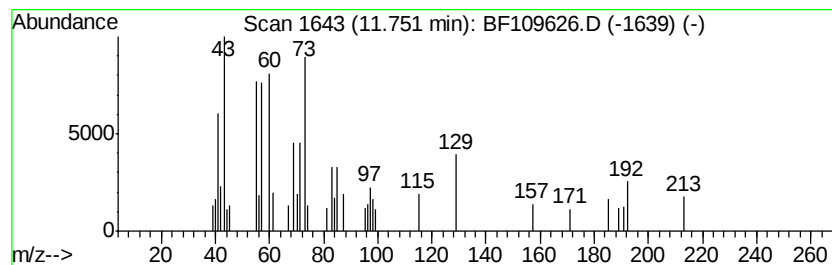
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	2.11 ng	56210	Phenanthrene-d10	11.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Undecanoic acid	186	C11H22O2	000112-37-8	64
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5		n-Decanoic acid	172	C10H20O2	000334-48-5	53



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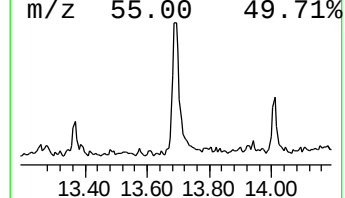
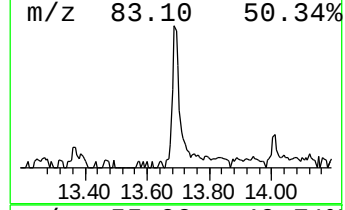
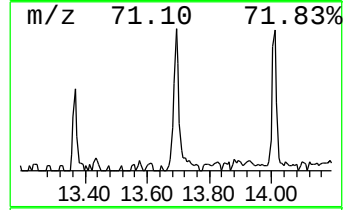
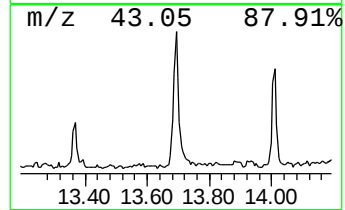
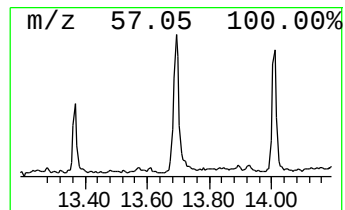
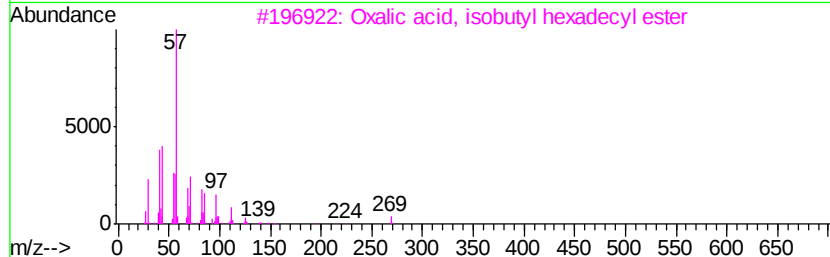
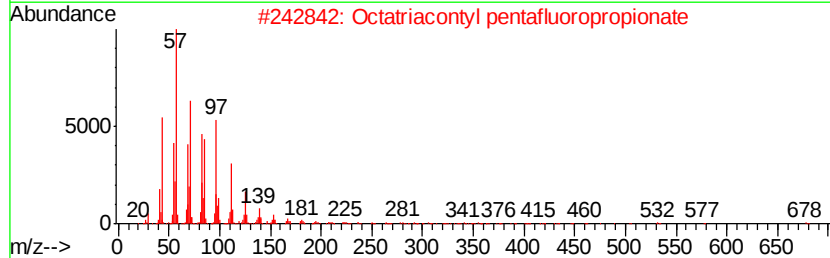
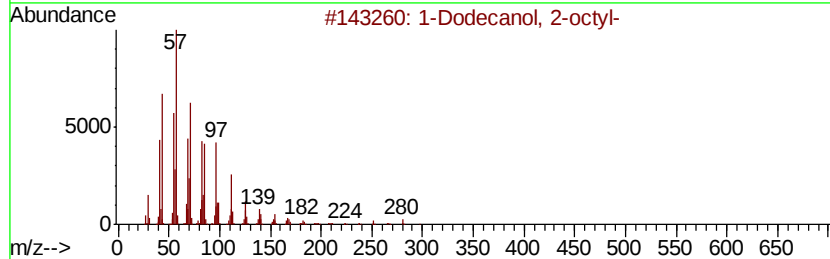
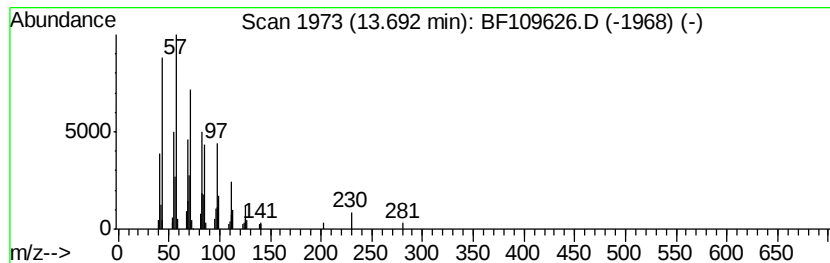
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Dodecanol, 2-octyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.69	4.87 ng	149955	Chrysene-d12	13.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
2	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	91
3	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
4	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	91
5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	87



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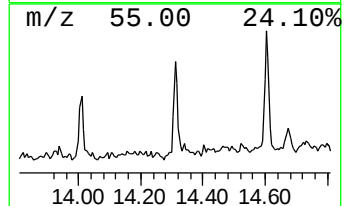
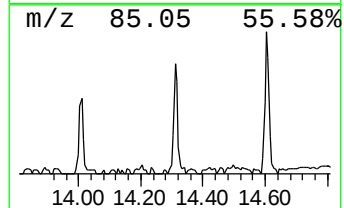
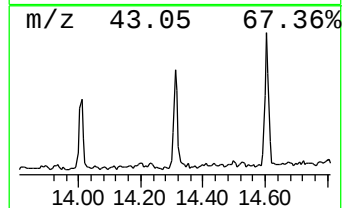
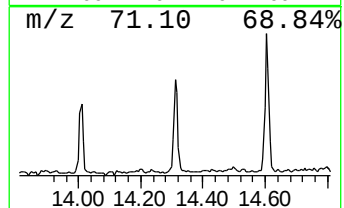
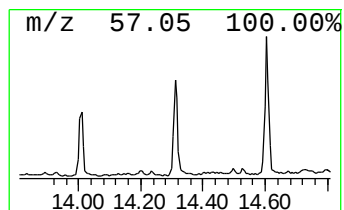
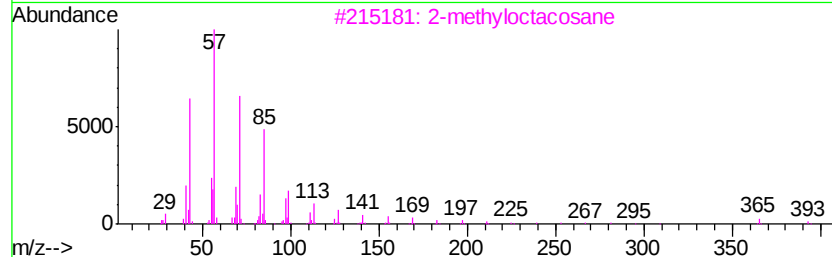
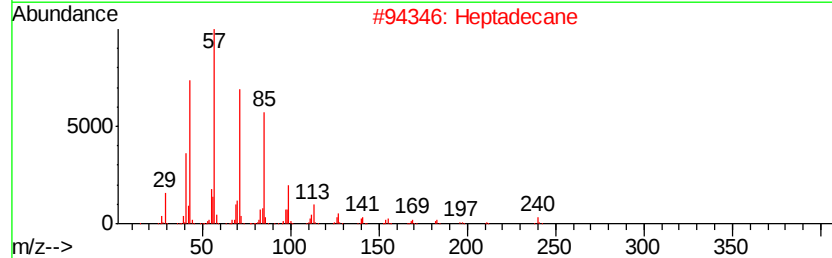
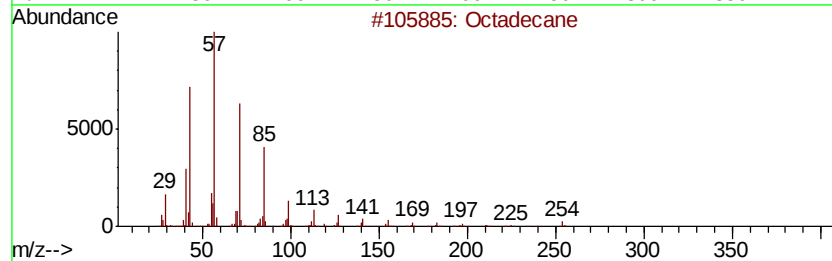
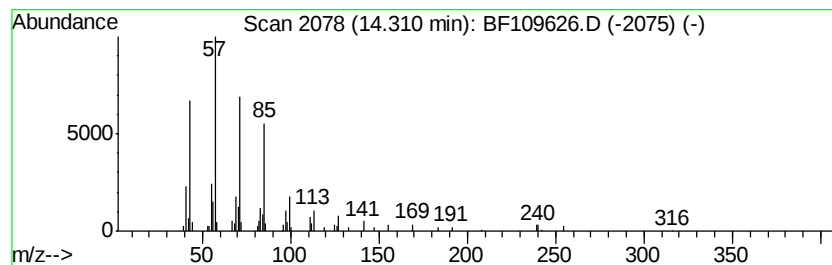
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.31	2.75 ng	84802	Chrysene-d12	13.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	96
2		Heptadecane	240	C17H36	000629-78-7	95
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Hexacosane	366	C26H54	000630-01-3	91



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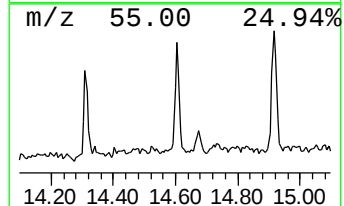
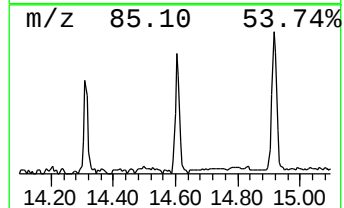
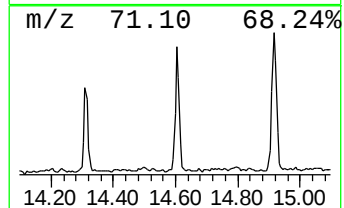
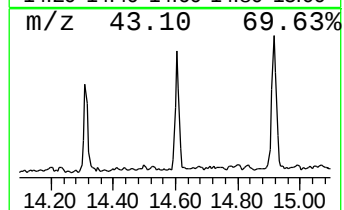
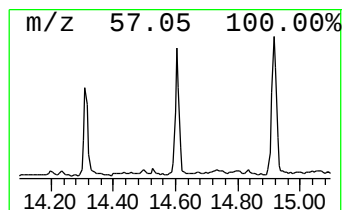
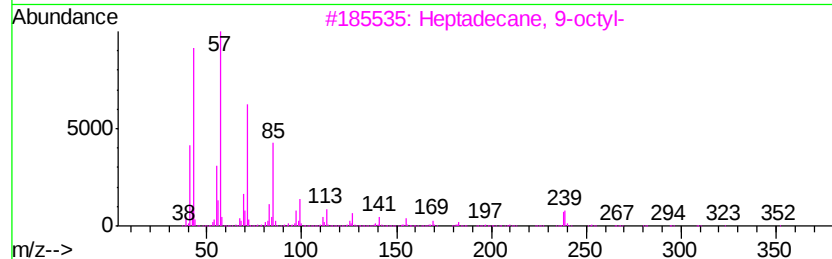
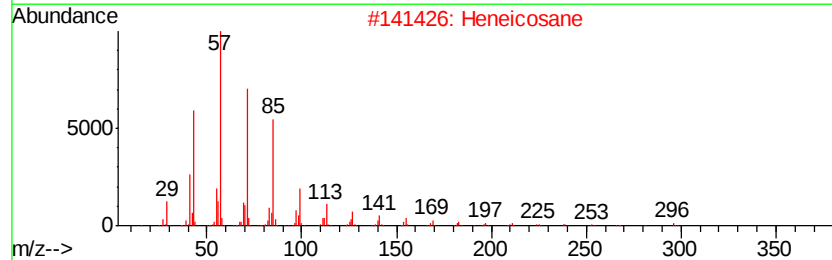
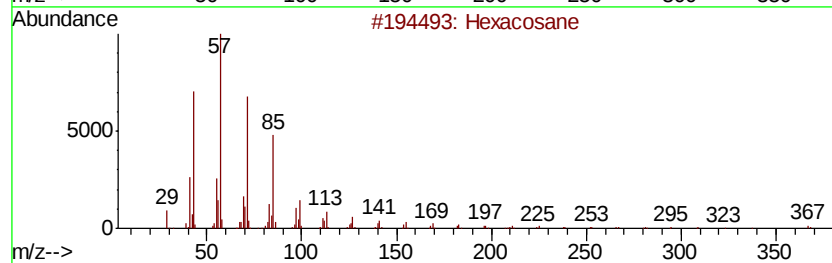
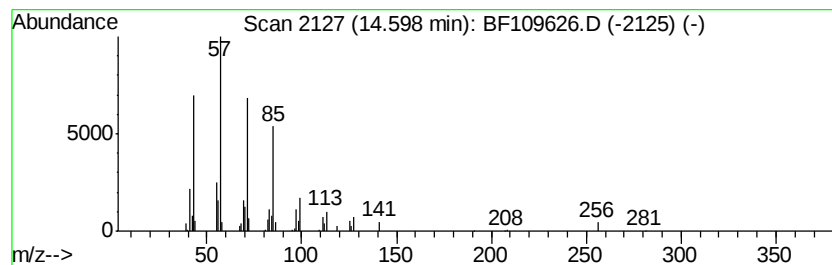
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	4.65 ng	114944	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Hexatriacontane	507	C36H74	000630-06-8	91



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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRID16-COMP-100318

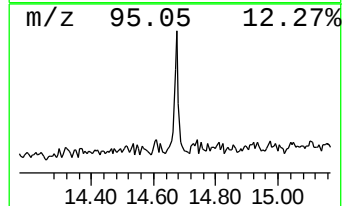
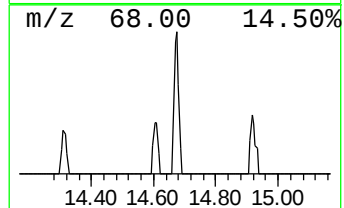
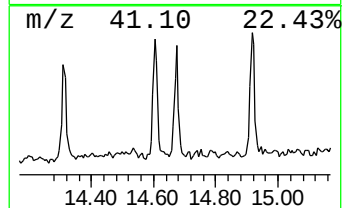
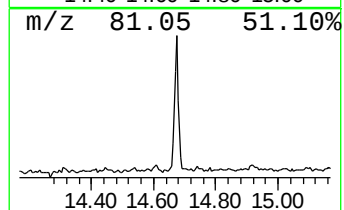
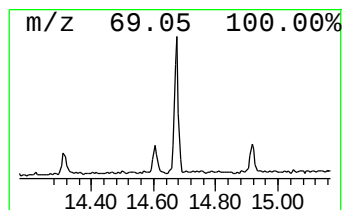
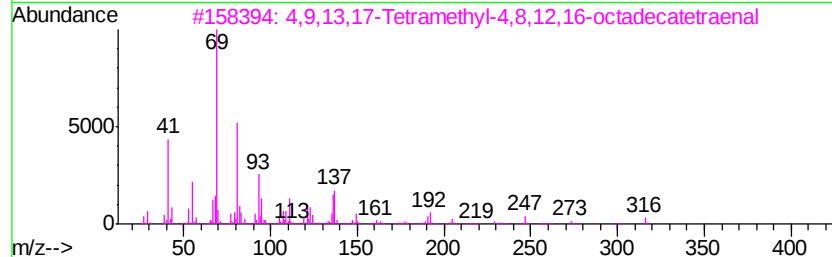
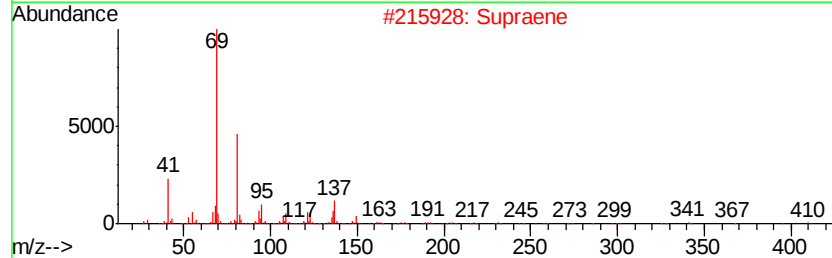
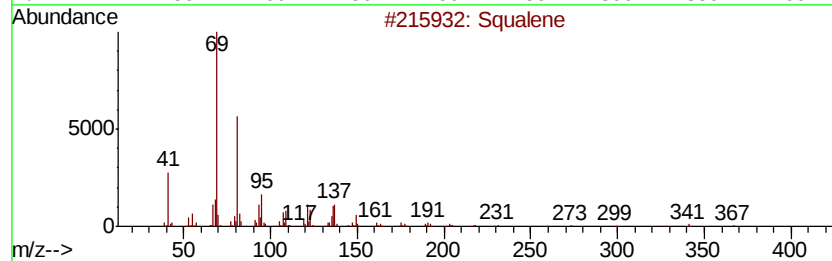
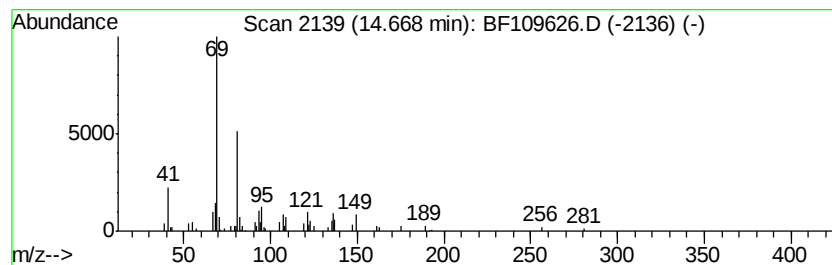
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	2.74 ng	67572	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	87
3		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
5		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100518\
Data File : BF109626.D
Acq On : 5 Oct 2018 23:24
Operator : JU/SJ
Sample : J5263-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRID16-COMP-100318

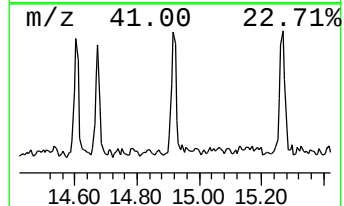
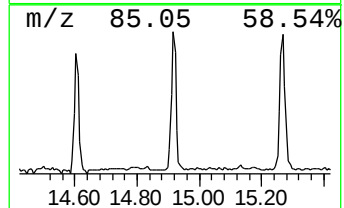
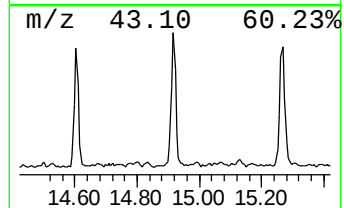
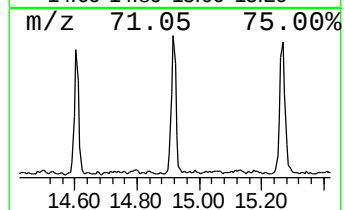
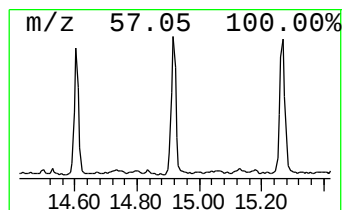
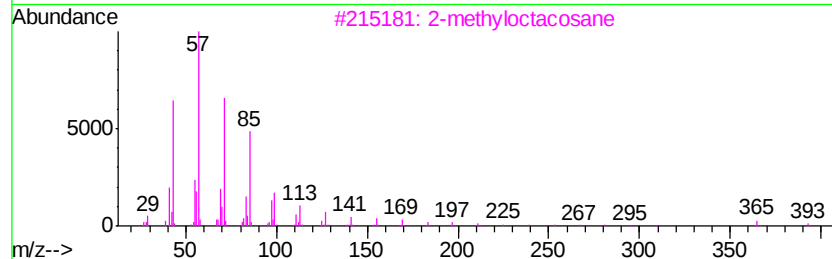
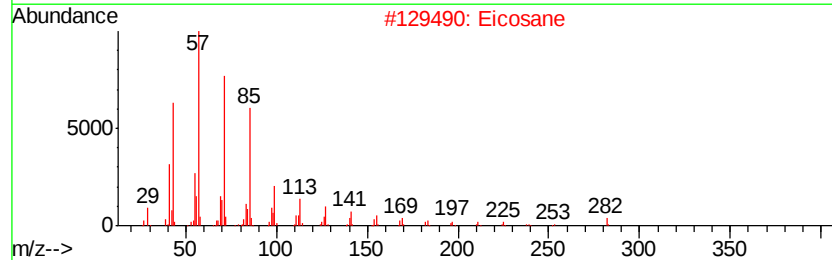
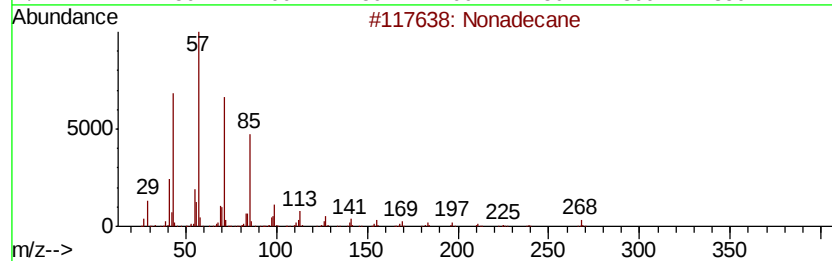
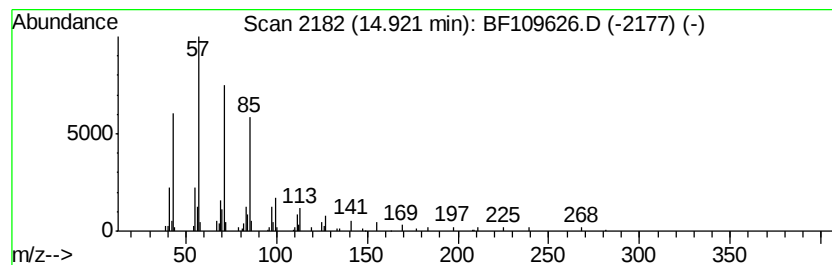
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	6.33 ng	156425	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	96
2		Eicosane	282	C20H42	000112-95-8	94
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100518\
Data File : BF109626.D
Acq On : 5 Oct 2018 23:24
Operator : JU/SJ
Sample : J5263-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRID16-COMP-100318

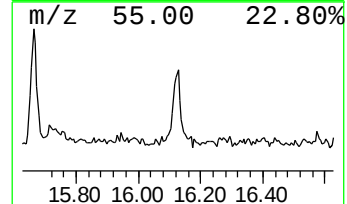
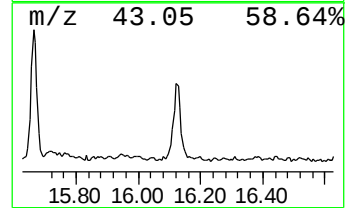
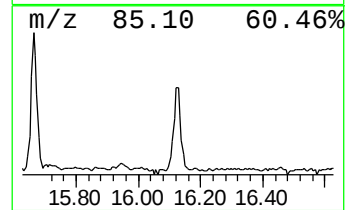
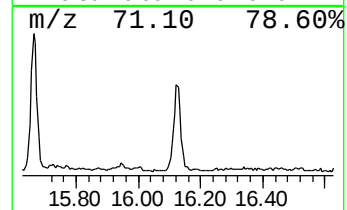
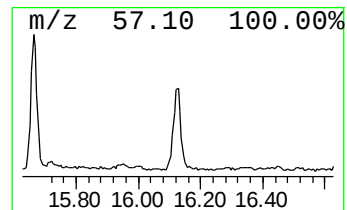
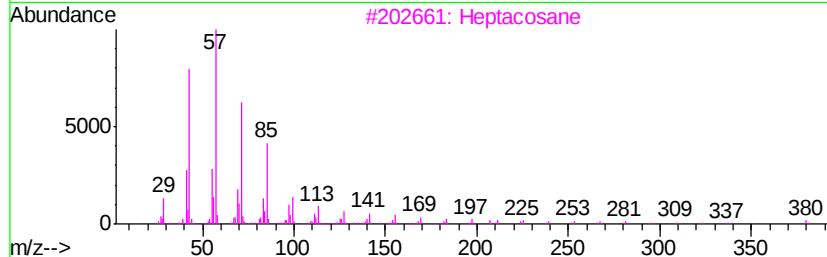
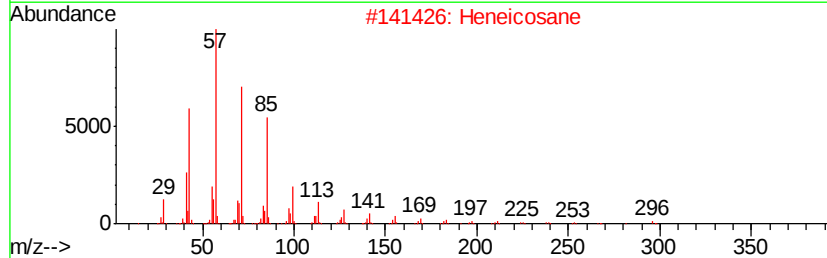
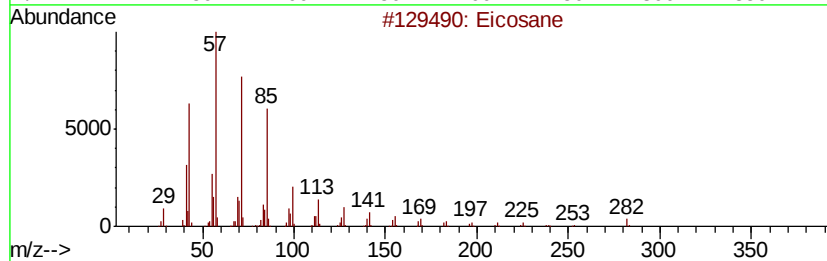
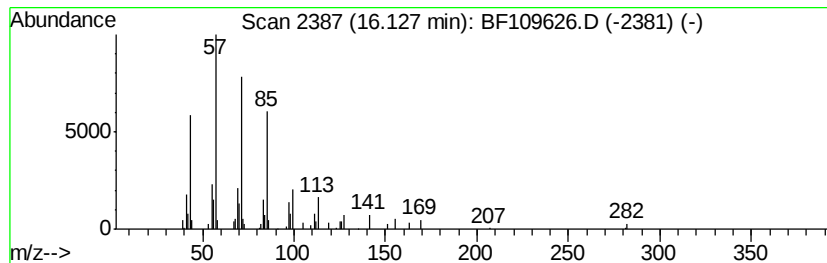
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	5.15 ng	127259	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	96
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		2-methyloctacosane	408	C29H60	1000376-72-8	91
5		Octacosane	394	C28H58	000630-02-4	91



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Acq On : 5 Oct 2018 23:24
Operator : JU/SJ
Sample : J5263-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRID16-COMP-100318

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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...	4.89	2.0	ng	47463	1	6.70	463026	20.0
n-Hexadecanoic acid	11.75	2.1	ng	56210	4	11.21	533296	20.0
1-Dodecanol, 2-oc...	13.69	4.9	ng	149955	5	13.83	616229	20.0
Octadecane	14.31	2.8	ng	84802	5	13.83	616229	20.0
Hexacosane	14.60	4.7	ng	114944	6	15.23	494125	20.0
Squalene	14.67	2.7	ng	67572	6	15.23	494125	20.0
Nonadecane	14.92	6.3	ng	156425	6	15.23	494125	20.0
Eicosane	16.13	5.2	ng	127259	6	15.23	494125	20.0