

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
 Data File : BF109386.D
 Acq On : 27 Sep 2018 14:53
 Operator : JU/SJ
 Sample : J5066-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP1-Q1-G3

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	4.898	474	478	486	rBV	51683	65608	2.95%	0.321%
2	5.316	545	549	553	rBV	1895233	1819773	81.87%	8.895%
3	6.345	719	724	729	rBV	2049804	2012240	90.52%	9.836%
4	6.475	742	746	749	rBV	2296408	1985280	89.31%	9.704%
5	6.704	782	785	789	rBV	813221	645139	29.02%	3.153%
6	6.863	808	812	815	rBV	1743734	1407540	63.32%	6.880%
7	6.981	829	832	838	rVB4	18515	28588	1.29%	0.140%
8	7.269	876	881	884	rVB	1232818	1206890	54.29%	5.899%
9	7.634	940	943	947	rVB2	26391	26810	1.21%	0.131%
10	7.987	999	1003	1011	rBV	1047763	851309	38.30%	4.161%
11	9.063	1182	1186	1189	rBV	2708312	2222892	100.00%	10.866%
12	9.457	1249	1253	1264	rBV	613558	501512	22.56%	2.451%
13	9.733	1297	1300	1304	rBV	1032487	949135	42.70%	4.639%
14	10.522	1430	1434	1441	rBV	1273501	1196560	53.83%	5.849%
15	11.210	1548	1551	1554	rBV	978712	907893	40.84%	4.438%
16	11.233	1554	1555	1559	rVB	42299	26359	1.19%	0.129%
17	11.751	1639	1643	1647	rBV3	33524	40205	1.81%	0.197%
18	12.416	1753	1756	1760	rVB	42478	38315	1.72%	0.187%
19	12.645	1789	1795	1798	rBV	40861	42433	1.91%	0.207%
20	12.792	1816	1820	1824	rBV	1824651	1737111	78.15%	8.491%
21	13.710	1969	1976	1986	rBV	121374	248404	11.17%	1.214%
22	13.839	1993	1998	2001	rBV	768811	700590	31.52%	3.425%
23	14.321	2077	2080	2083	rBV	47040	47110	2.12%	0.230%
24	14.615	2128	2130	2138	rVB	79677	81141	3.65%	0.397%
25	14.839	2166	2168	2178	rVB	25728	55098	2.48%	0.269%
26	14.933	2180	2184	2189	rVV	110318	123227	5.54%	0.602%
27	15.239	2231	2236	2240	rBV	659175	750173	33.75%	3.667%
28	15.286	2240	2244	2251	rVB	143260	172817	7.77%	0.845%
29	15.686	2307	2312	2319	rBV	135785	194180	8.74%	0.949%
30	16.145	2385	2390	2401	rVB2	98012	173658	7.81%	0.849%
31	16.686	2476	2482	2488	rBV3	47959	103572	4.66%	0.506%
32	17.327	2587	2591	2598	rVB4	29886	59011	2.65%	0.288%
33	18.080	2715	2719	2727	rVB8	15975	37366	1.68%	0.183%

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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q1-G3

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

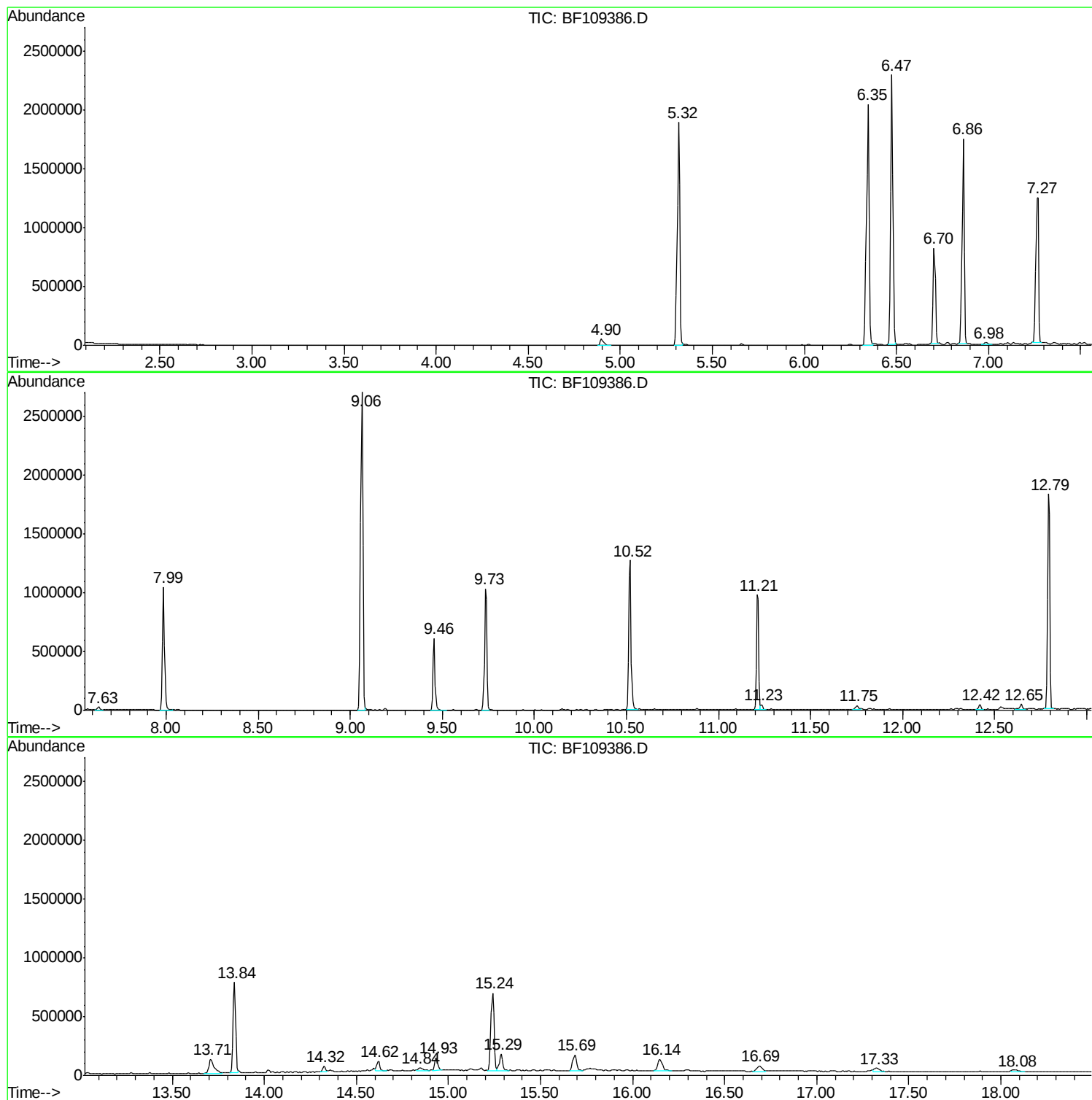
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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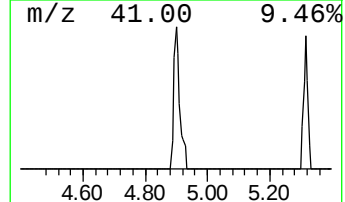
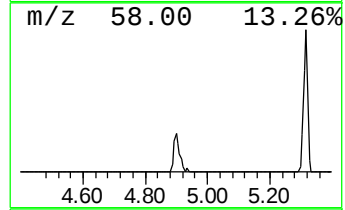
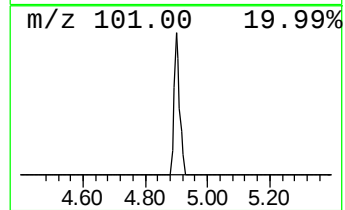
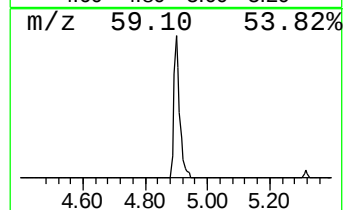
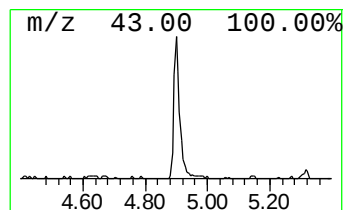
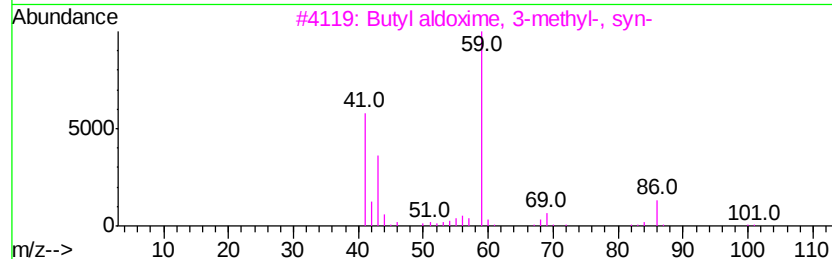
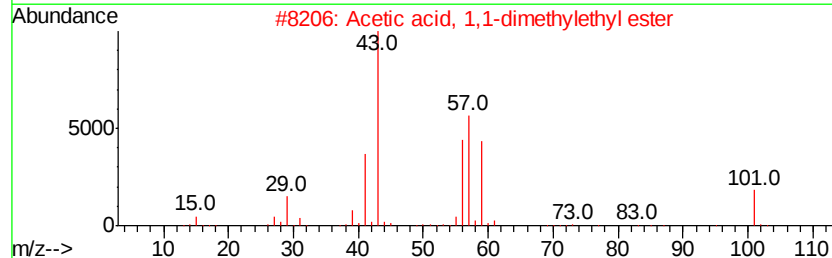
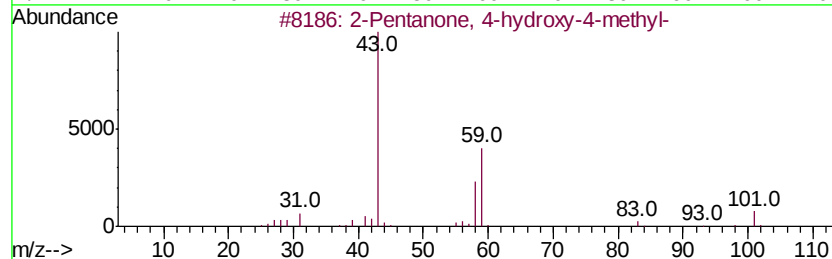
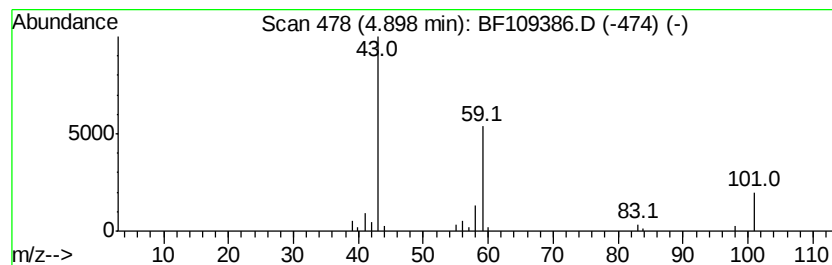
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	2.03 ng	65608	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	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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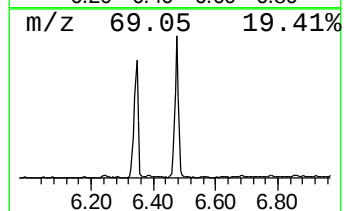
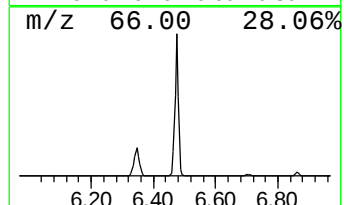
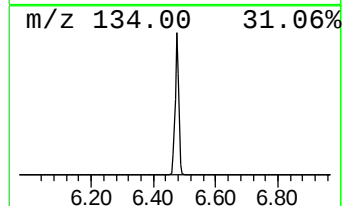
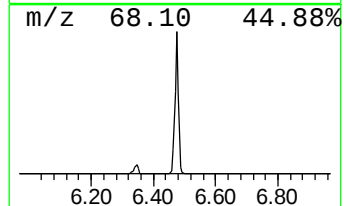
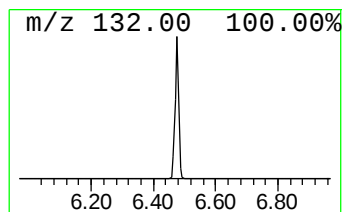
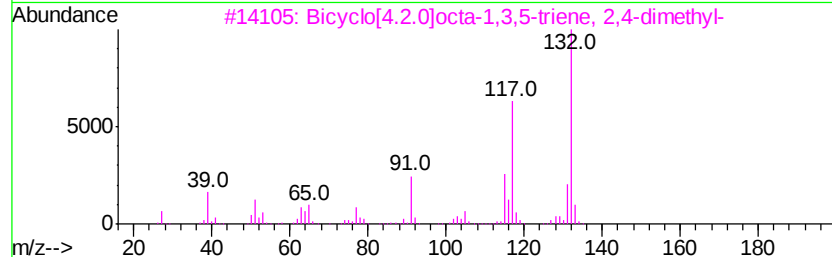
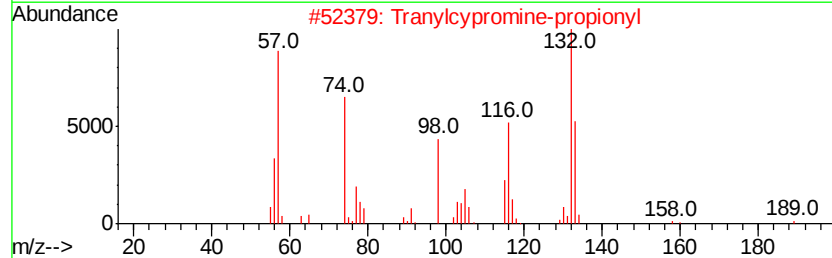
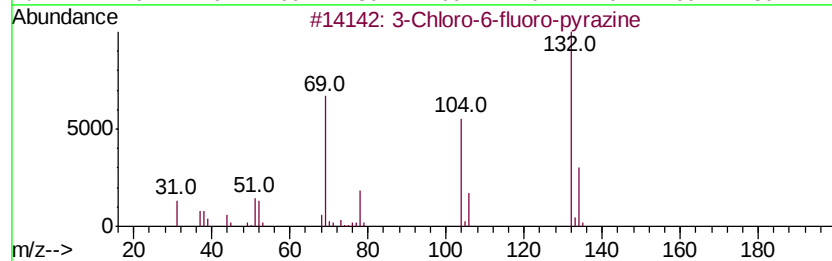
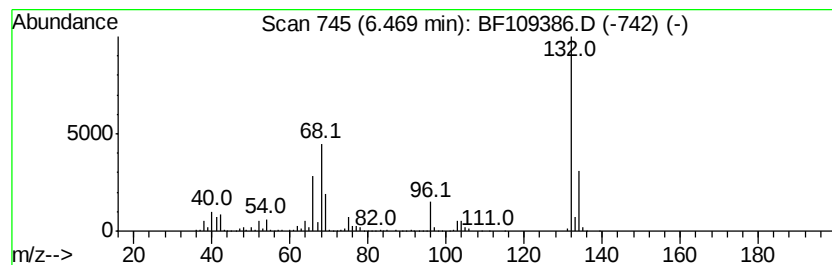
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	61.55 ng	1985280	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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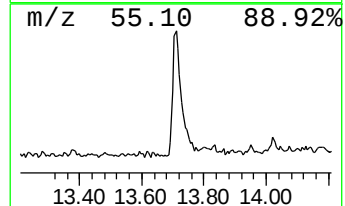
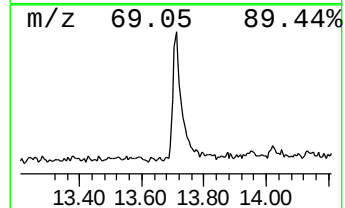
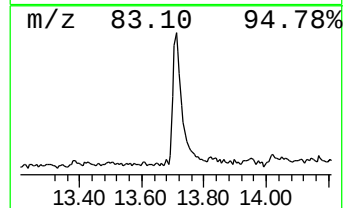
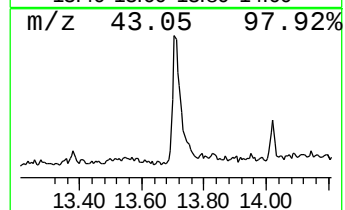
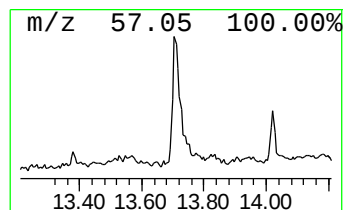
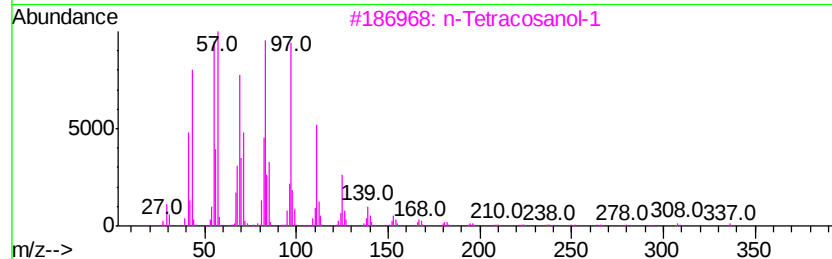
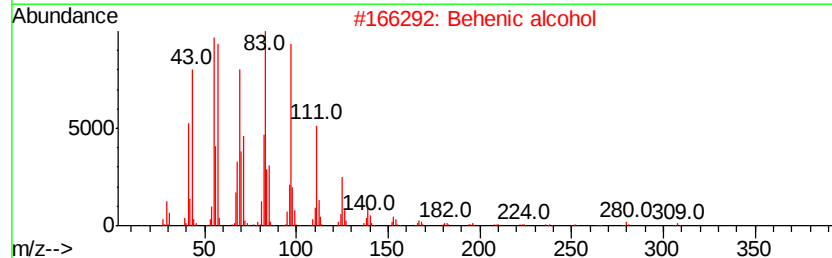
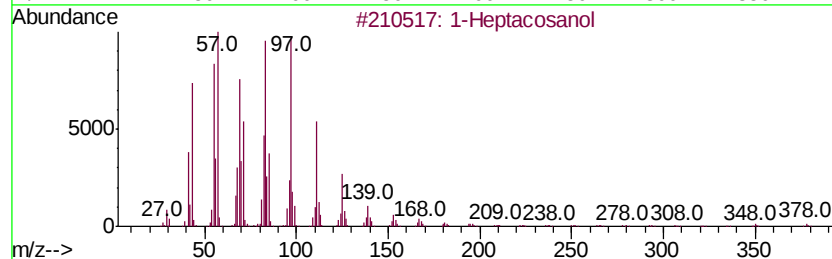
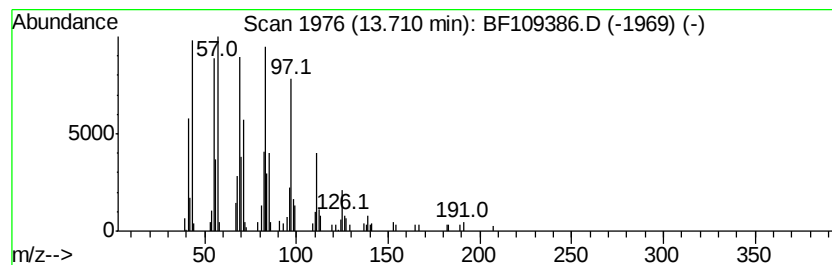
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Heptacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	7.09 ng	248404	Chrysene-d12	13.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heptacosanol	396	C27H56O	002004-39-9	93
2		Behenic alcohol	326	C22H46O	000661-19-8	93
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4		1-Heneicosanol	312	C21H44O	015594-90-8	93
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	90



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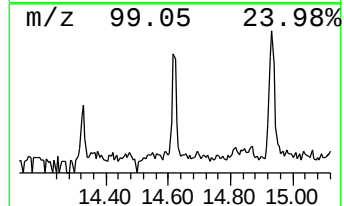
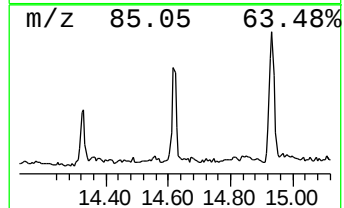
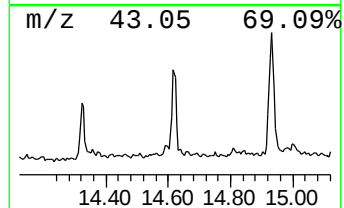
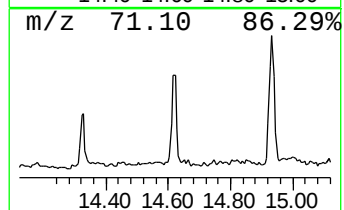
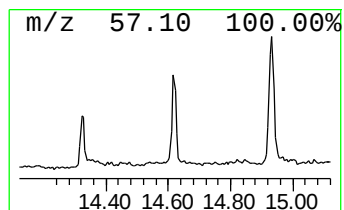
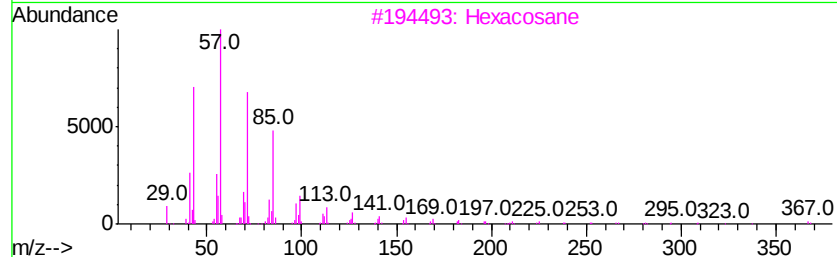
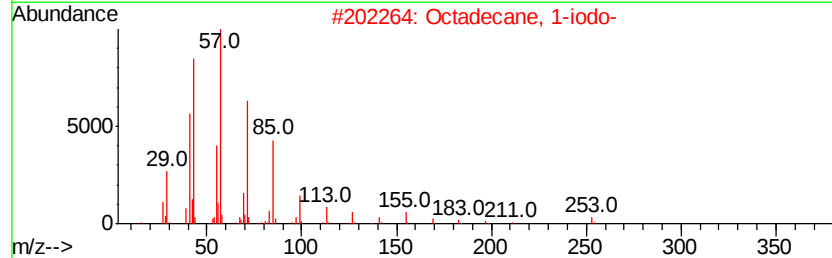
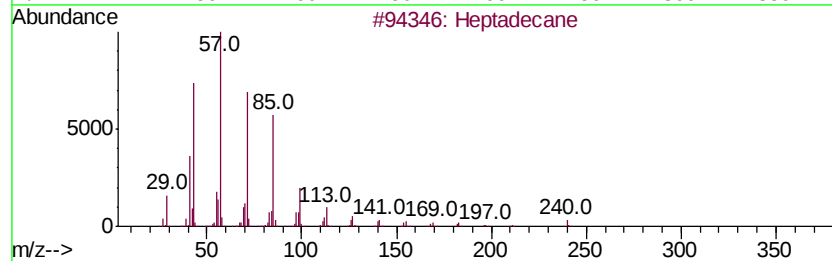
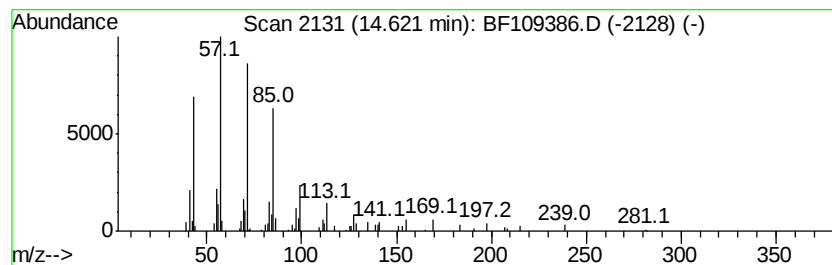
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.16 ng	81141	Perylene-d12	15.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	86
2	Octadecane, 1-iodo-		380	C18H37I	000629-93-6	86
3	Hexacosane		366	C26H54	000630-01-3	80
4	Tetratetracontane		619	C44H90	007098-22-8	74
5	2-Bromo dodecane		248	C12H25Br	013187-99-0	72



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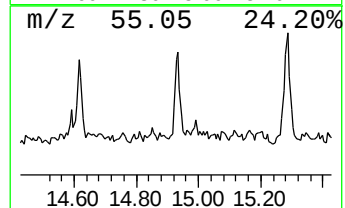
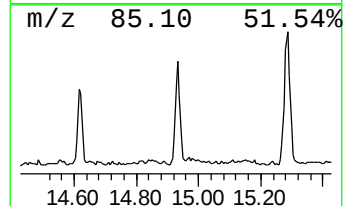
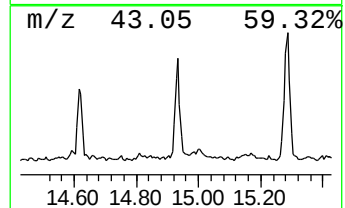
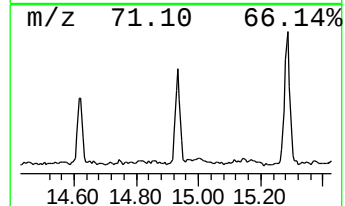
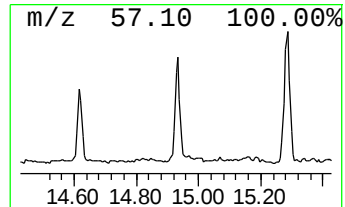
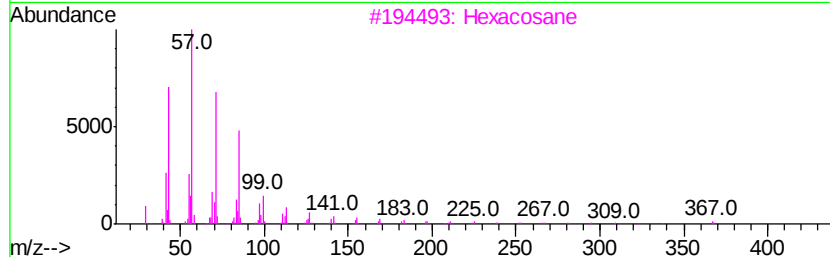
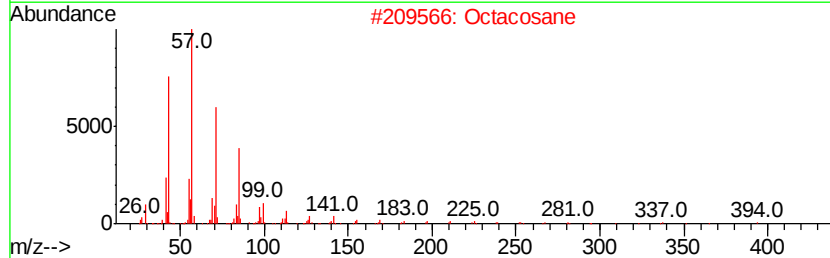
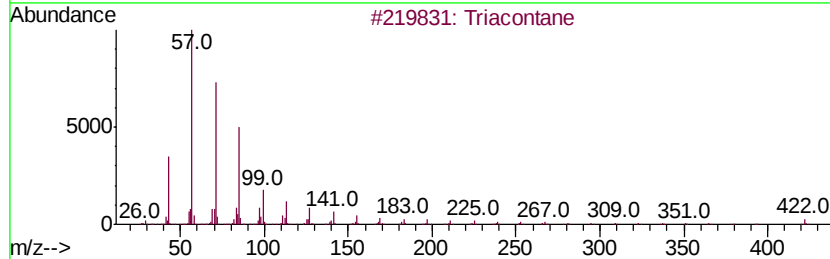
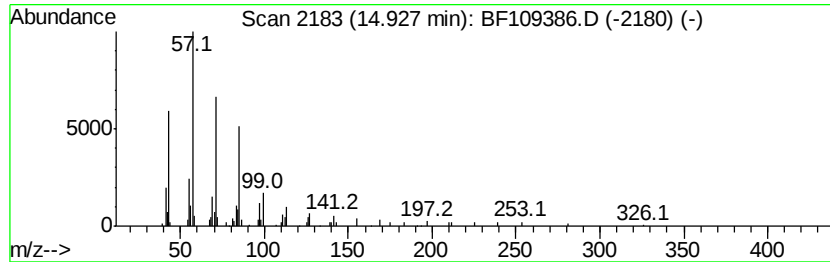
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Peak Number 6 Triacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	3.29 ng	123227	Perylene-d12	15.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Heneicosane	296	C21H44	000629-94-7	91



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ClientSampleId :
EP1-Q1-G3

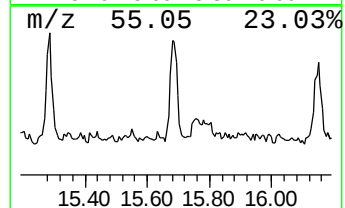
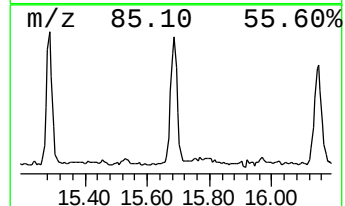
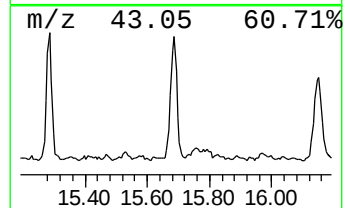
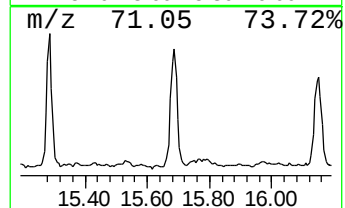
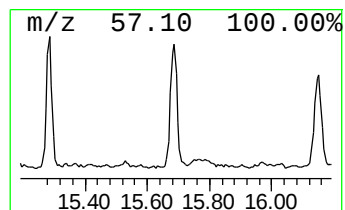
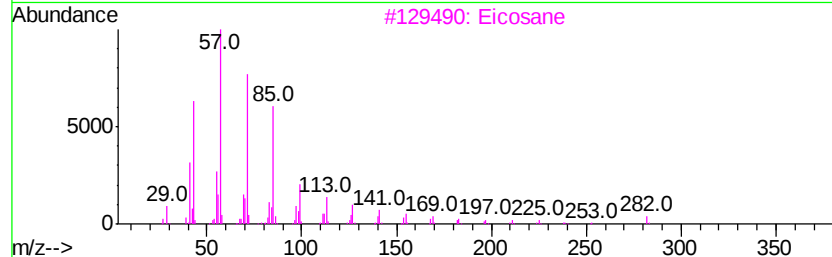
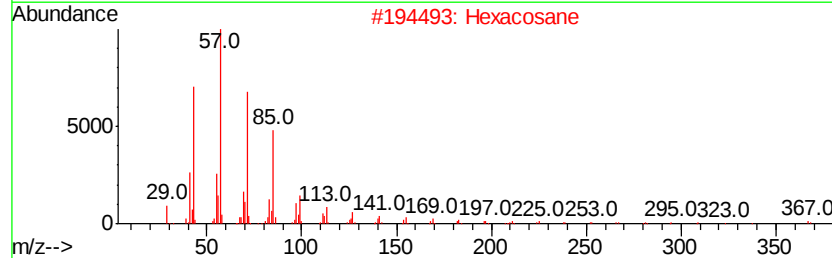
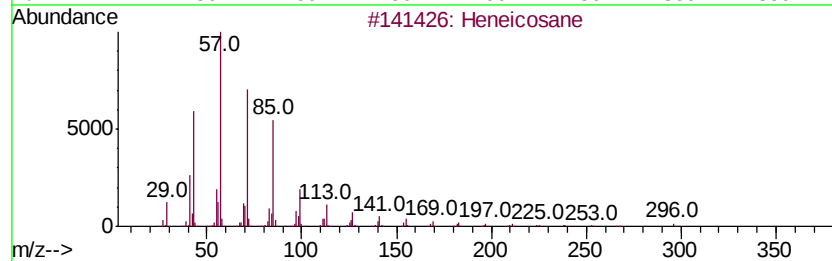
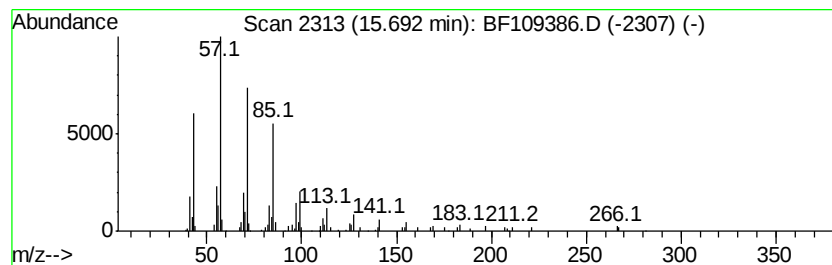
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	5.18 ng	194180	Perylene-d12	15.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Hexacosane		366	C26H54	000630-01-3	91
3	Eicosane		282	C20H42	000112-95-8	91
4	2-methyloctacosane		408	C29H60	1000376-72-8	91
5	Triacontane		422	C30H62	000638-68-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
Data File : BF109386.D
Acq On : 27 Sep 2018 14:53
Operator : JU/SJ
Sample : J5066-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q1-G3

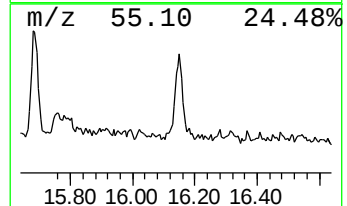
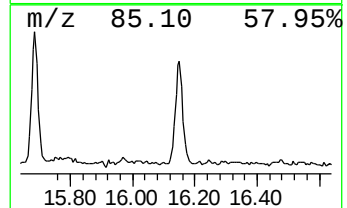
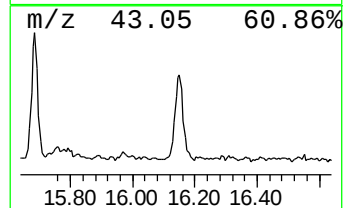
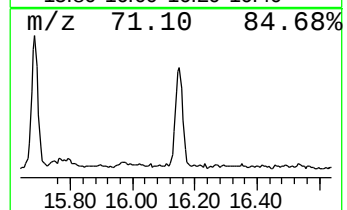
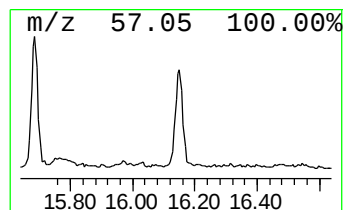
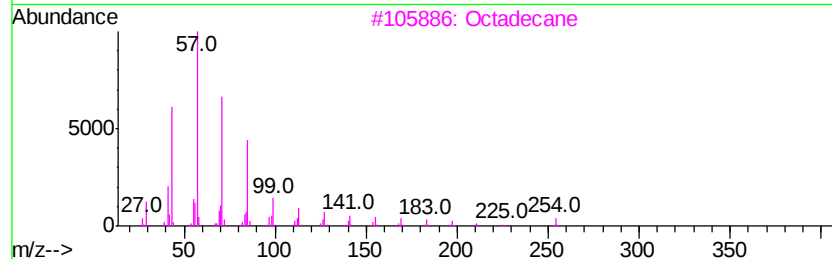
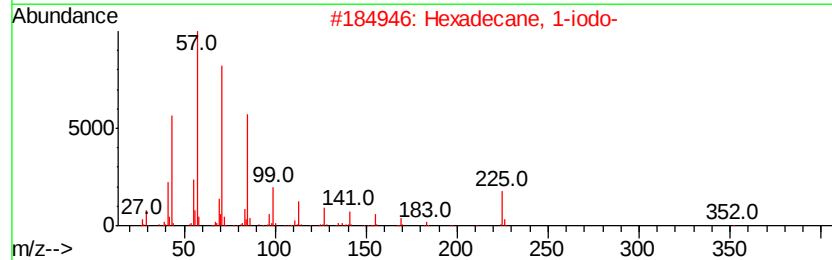
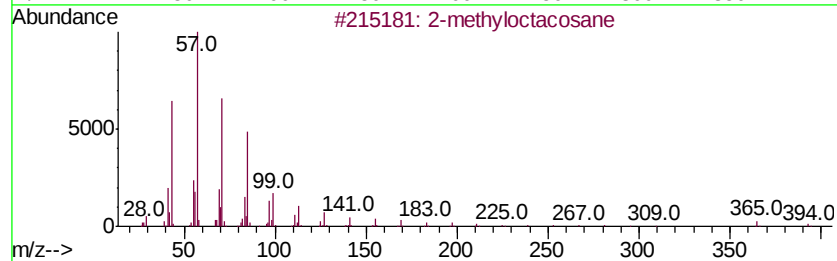
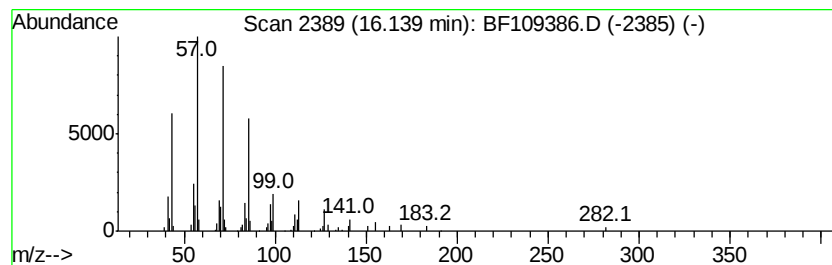
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.14	4.63 ng	173658	Perylene-d12	15.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	91
3		Octadecane	254	C18H38	000593-45-3	91
4		triacontane	422	C30H62	000638-68-6	91
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
Data File : BF109386.D
Acq On : 27 Sep 2018 14:53
Operator : JU/SJ
Sample : J5066-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q1-G3

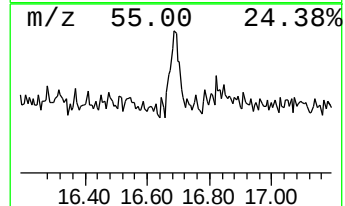
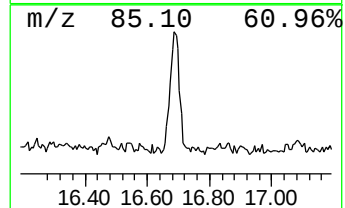
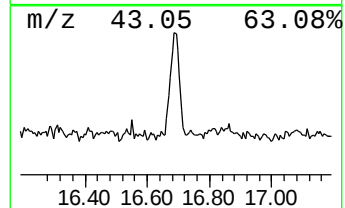
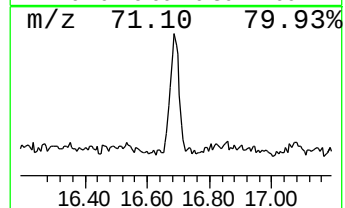
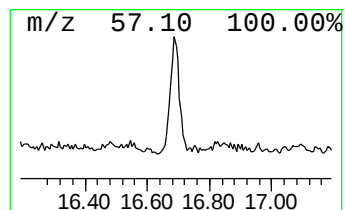
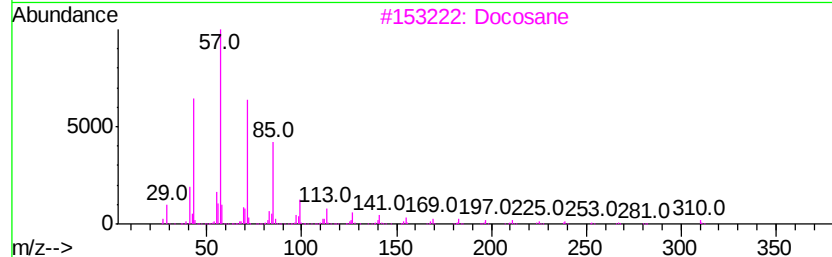
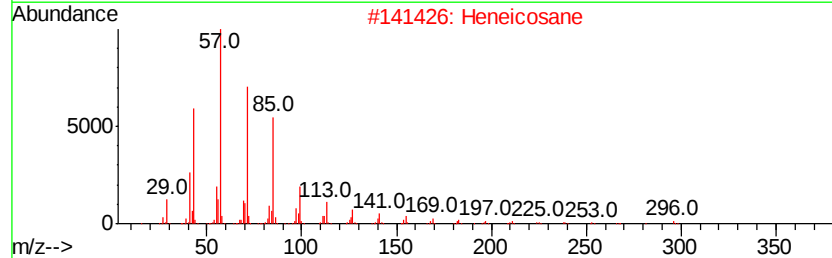
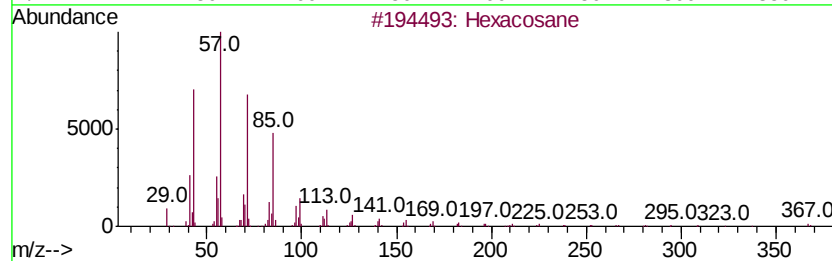
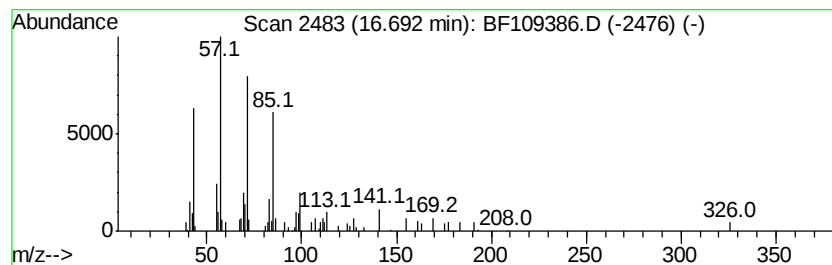
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.69	2.76 ng	103572	Perylene-d12	15.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	83
2	Heneicosane		296	C21H44	000629-94-7	83
3	Docosane		310	C22H46	000629-97-0	80
4	Eicosane		282	C20H42	000112-95-8	76
5	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092718\
Data File : BF109386.D
Acq On : 27 Sep 2018 14:53
Operator : JU/SJ
Sample : J5066-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q1-G3

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
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unknown6.47	6.47	61.5	ng	1985280	1	6.70	645139	20.0
1-Heptacosanol	13.71	7.1	ng	248404	5	13.84	700590	20.0
Heptadecane	14.62	2.2	ng	81141	6	15.24	750173	20.0
triacontane	14.93	3.3	ng	123227	6	15.24	750173	20.0
Heneicosane	15.69	5.2	ng	194180	6	15.24	750173	20.0
2-methyloctacosane	16.14	4.6	ng	173658	6	15.24	750173	20.0
Hexacosane	16.69	2.8	ng	103572	6	15.24	750173	20.0