

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF011419\
 Data File : BF112049.D
 Acq On : 14 Jan 2019 14:37
 Operator : JU/SJ
 Sample : K1128-03
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RBR-200036

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-BF010719.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	2.152	8	11	25	rVB	66803	117643	4.05%	0.440%
2	5.081	506	509	519	rVB	131701	154635	5.32%	0.579%
3	5.504	577	581	584	rBV	3008059	2642965	90.96%	9.891%
4	6.510	747	752	763	rBV	2926772	2891088	99.50%	10.819%
5	6.645	770	775	778	rBV	3169734	2905644	100.00%	10.874%
6	6.692	780	783	793	rVB	49175	63450	2.18%	0.237%
7	6.869	809	813	816	rBV	926499	798778	27.49%	2.989%
8	7.022	835	839	843	rBV	2143691	1958251	67.39%	7.328%
9	7.428	903	908	911	rBV	1815994	1645091	56.62%	6.156%
10	8.151	1026	1031	1034	rBV	1460311	1318112	45.36%	4.933%
11	9.222	1209	1213	1216	rBV	2406722	1934609	66.58%	7.240%
12	9.616	1276	1280	1283	rBV	837557	705004	24.26%	2.638%
13	9.904	1325	1329	1333	rBV	1355798	1162032	39.99%	4.349%
14	10.698	1459	1464	1467	rBV	2002423	1909832	65.73%	7.147%
15	10.822	1479	1485	1491	rVB5	27456	39952	1.37%	0.150%
16	10.875	1491	1494	1496	rBV	39298	32773	1.13%	0.123%
17	10.904	1496	1499	1503	rVB3	31654	36350	1.25%	0.136%
18	11.092	1527	1531	1533	rBV	47104	47695	1.64%	0.178%
19	11.392	1578	1582	1585	rBV	1536755	1278065	43.99%	4.783%
20	11.916	1668	1671	1679	rVB3	55001	58096	2.00%	0.217%
21	12.433	1755	1759	1763	rBV5	22104	36320	1.25%	0.136%
22	12.474	1763	1766	1770	rVB	40305	36514	1.26%	0.137%
23	12.604	1785	1788	1793	rVB	59222	55870	1.92%	0.209%
24	12.851	1822	1830	1831	rBV3	83706	123506	4.25%	0.462%
25	12.869	1831	1833	1838	rVB	90439	73348	2.52%	0.274%
26	12.974	1847	1851	1855	rVB	2159532	1849882	63.67%	6.923%
27	13.204	1887	1890	1893	rBV	79346	60064	2.07%	0.225%
28	13.433	1925	1929	1936	rBV5	38828	66477	2.29%	0.249%
29	13.545	1946	1948	1950	rBV	111828	80665	2.78%	0.302%
30	13.874	2000	2004	2010	rVB	177777	198492	6.83%	0.743%
31	14.033	2027	2031	2034	rBV	1015818	877489	30.20%	3.284%
32	14.192	2054	2058	2063	rBV	131173	133262	4.59%	0.499%
33	14.492	2106	2109	2113	rBV	133976	128985	4.44%	0.483%
34	14.804	2159	2162	2166	rVB	116657	113781	3.92%	0.426%

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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

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35	15.145	2216	2220	2225	rVB	98427	122406	4.21%	0.458%
36	15.510	2277	2282	2292	rVB2	645312	913790	31.45%	3.420%
37	15.963	2356	2359	2364	rVB	54887	83014	2.86%	0.311%
38	16.474	2443	2446	2451	rVB2	45264	67404	2.32%	0.252%

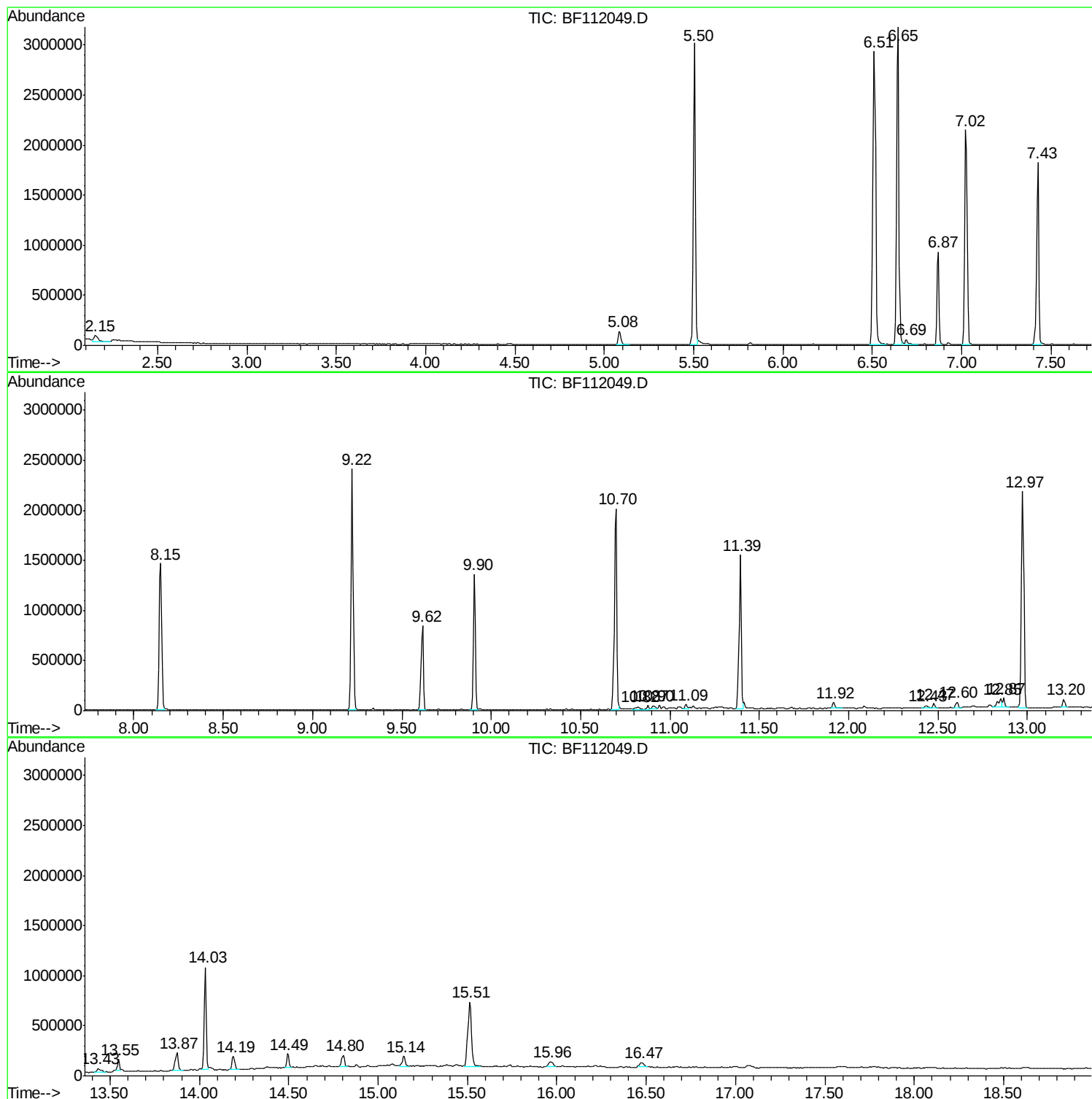
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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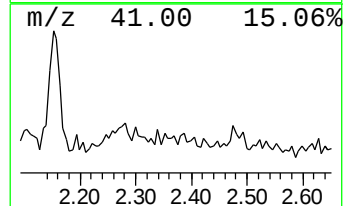
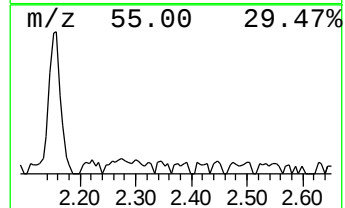
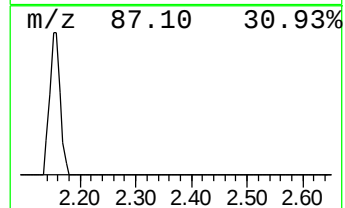
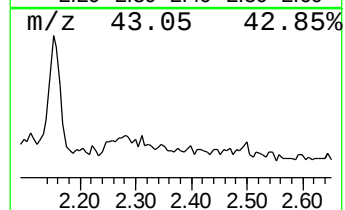
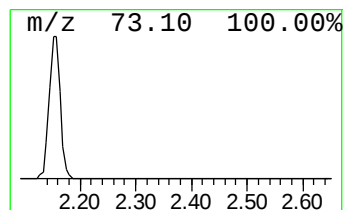
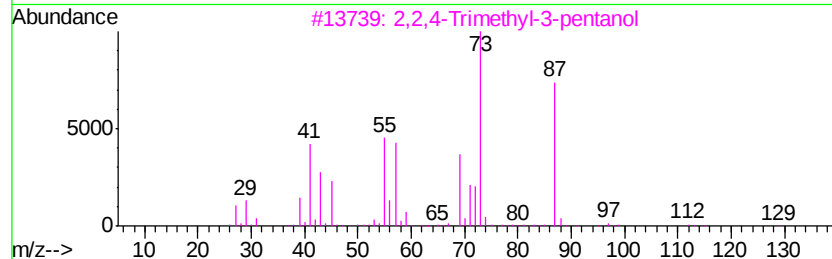
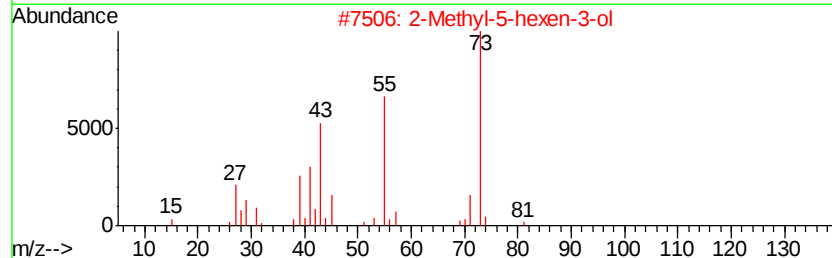
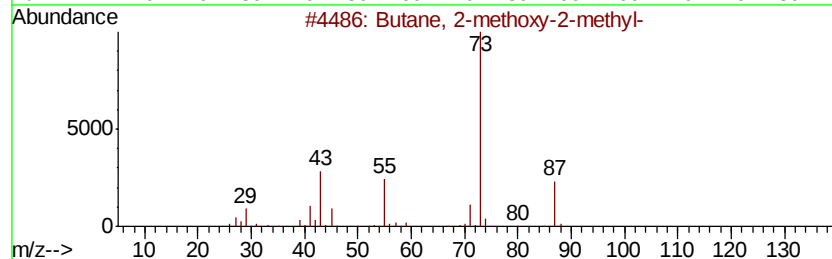
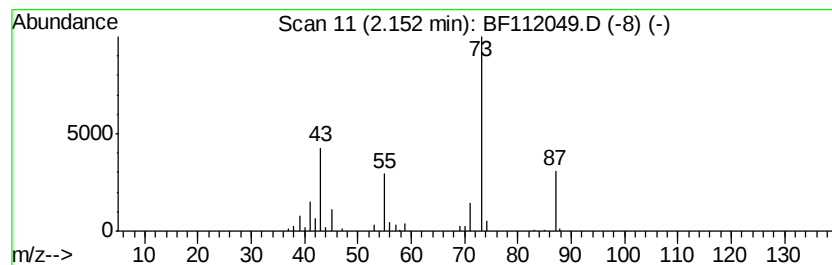
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	2.95 ng	117643	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	43
3		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	10



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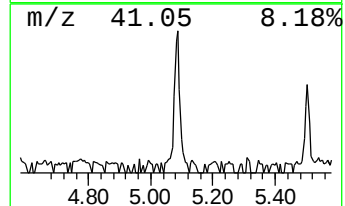
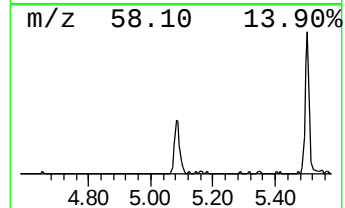
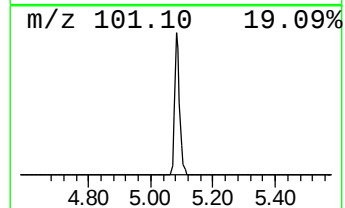
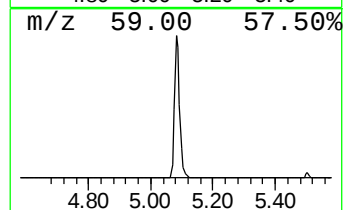
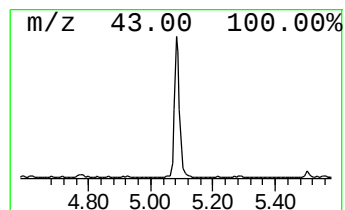
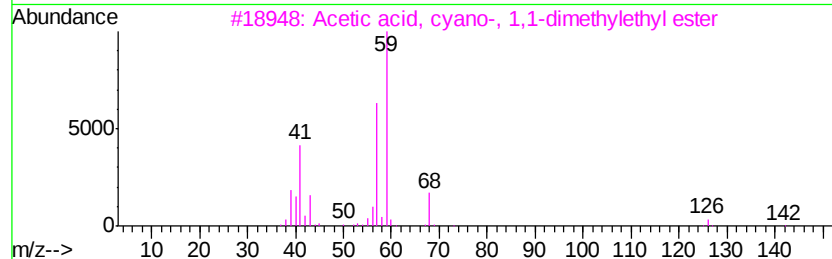
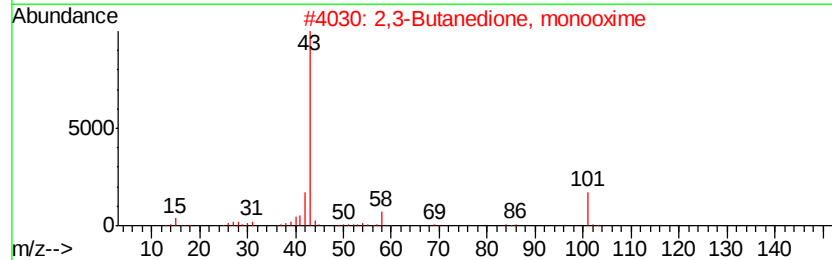
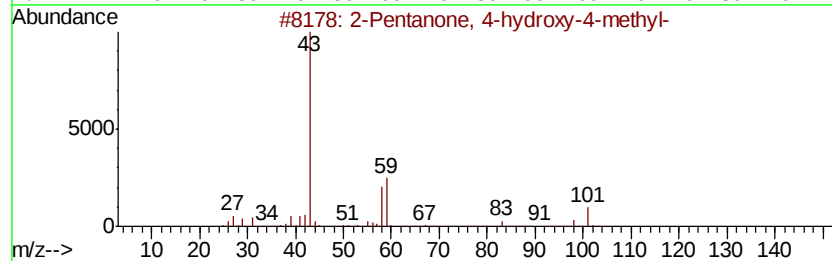
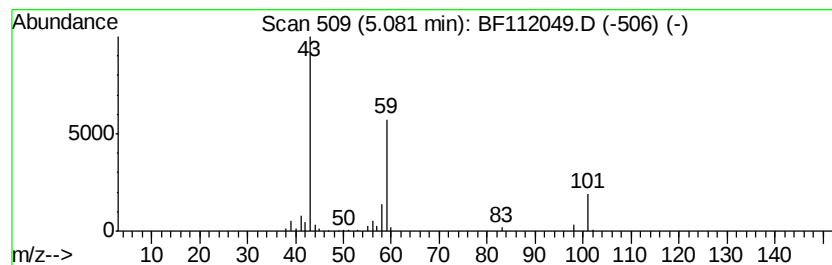
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	3.87 ng	154635	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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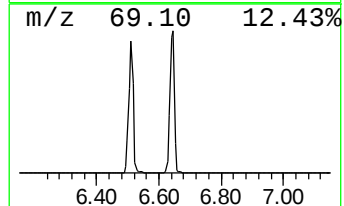
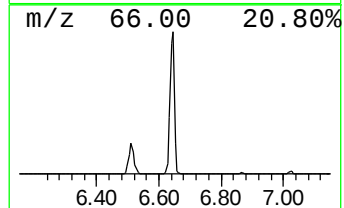
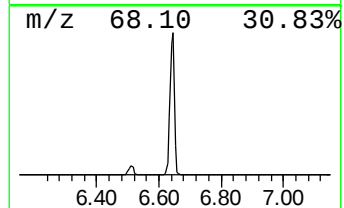
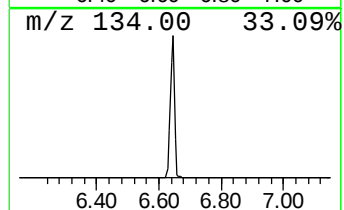
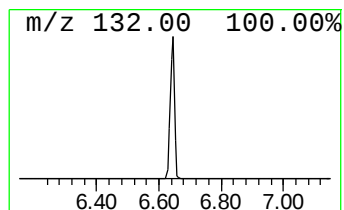
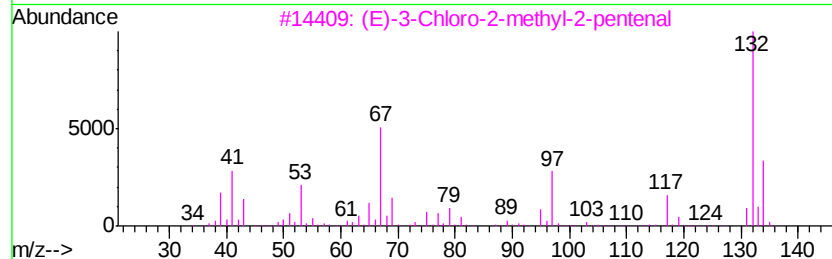
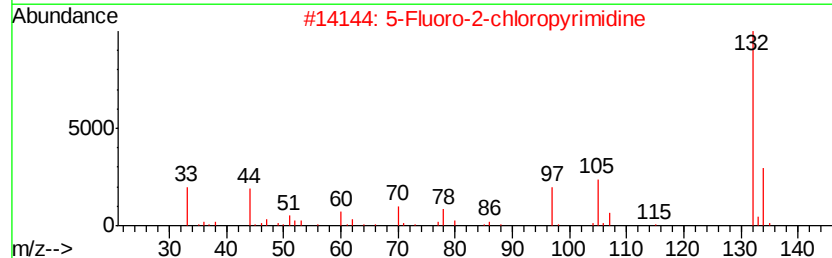
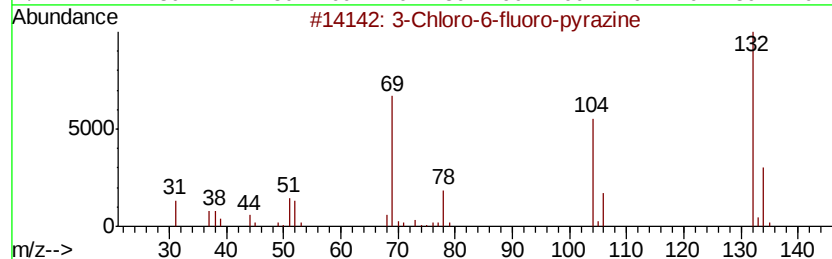
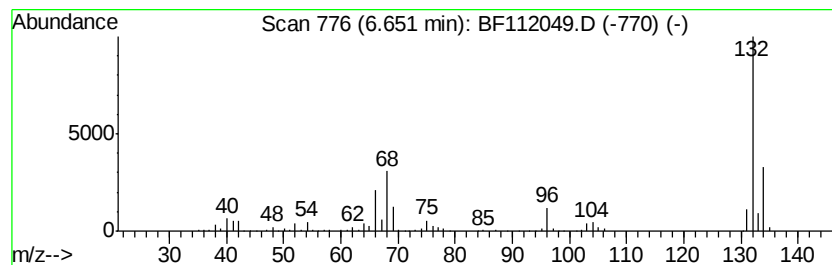
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	72.75 ng	2905640	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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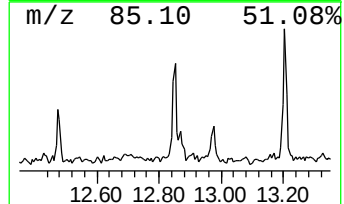
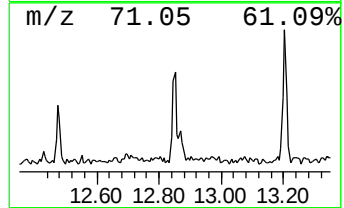
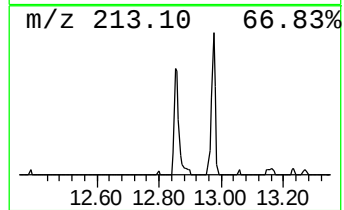
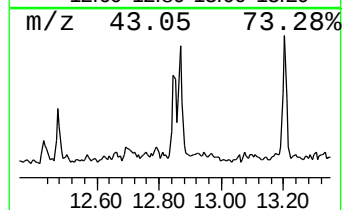
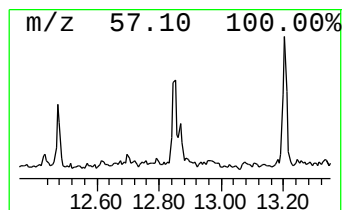
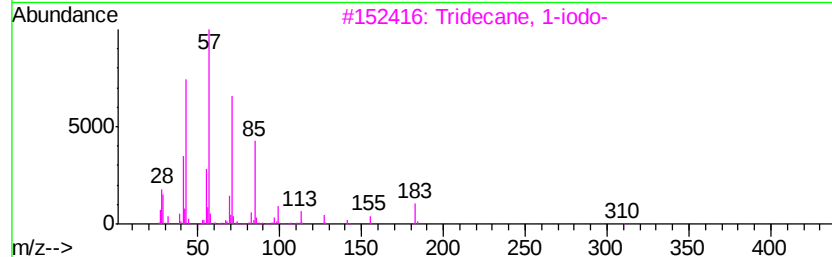
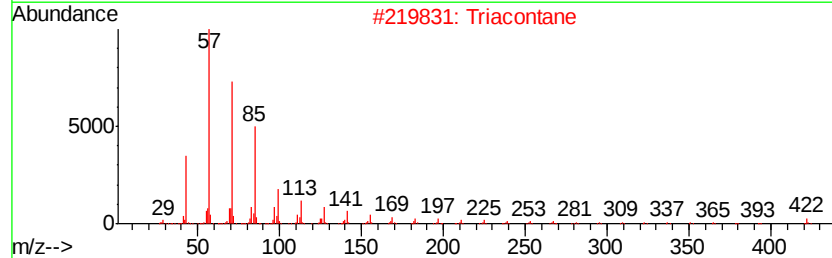
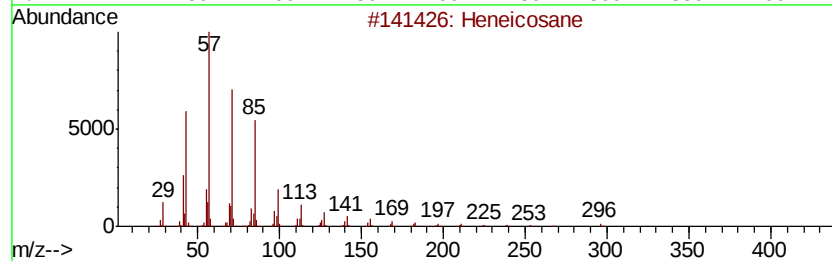
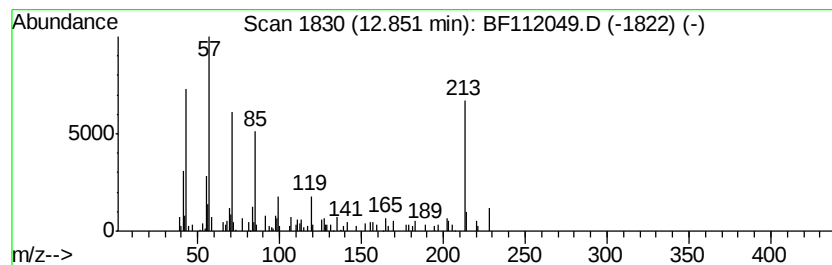
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown12.85 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.85	2.81 ng	123506	Chrysene-d12	14.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	49
2		Triacontane	422	C30H62	000638-68-6	46
3		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	46
4		Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	43
5		Hexacosane	366	C26H54	000630-01-3	41



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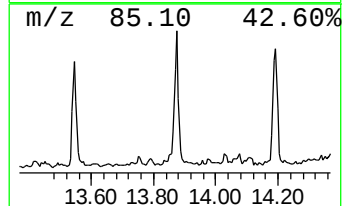
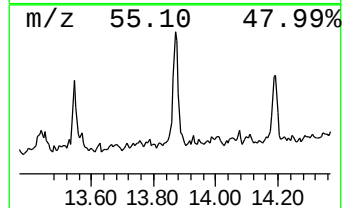
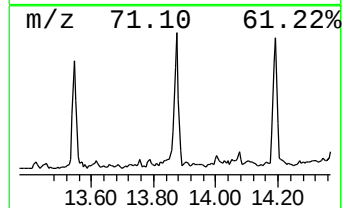
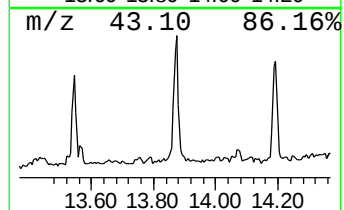
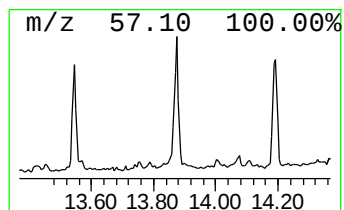
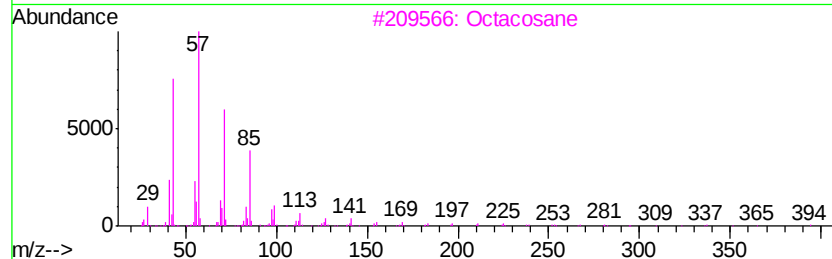
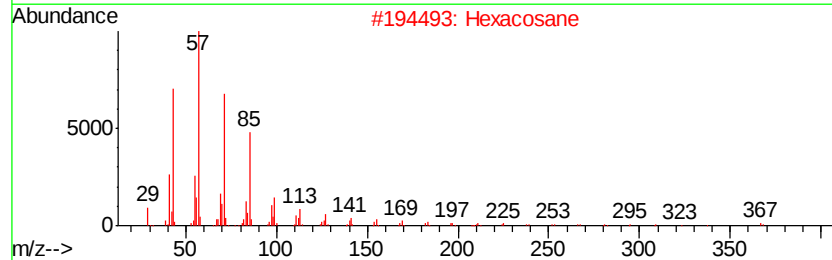
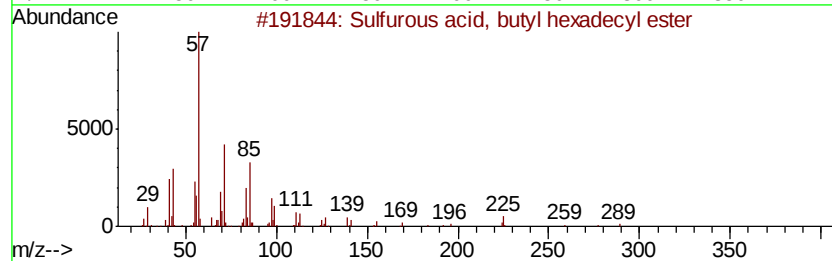
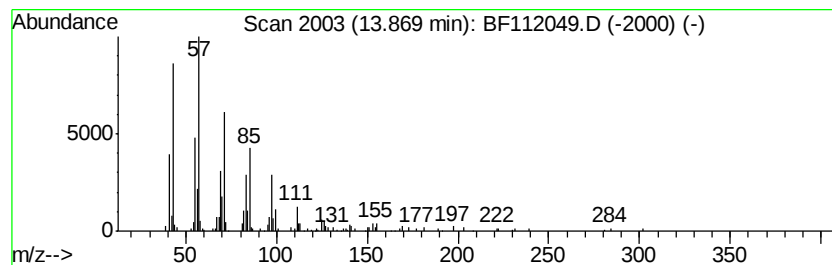
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Sulfurous acid, butyl hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	4.52 ng	198492	Chrysene-d12	14.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	91
2		Hexacosane	366	C26H54	000630-01-3	90
3		Octacosane	394	C28H58	000630-02-4	90
4		Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	90
5		2-methyloctacosane	408	C29H60	1000376-72-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011419\
Data File : BF112049.D
Acq On : 14 Jan 2019 14:37
Operator : JU/SJ
Sample : K1128-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-200036

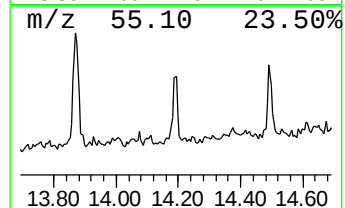
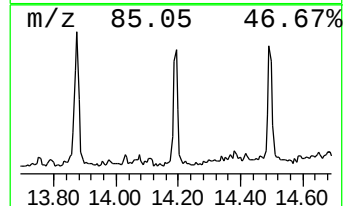
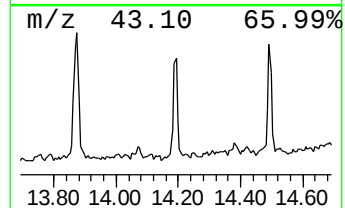
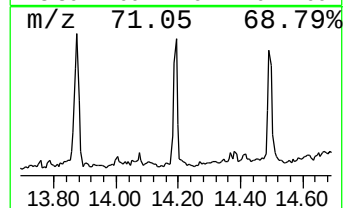
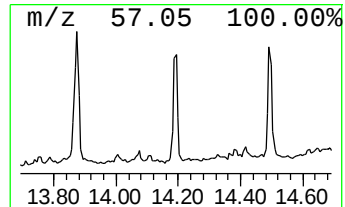
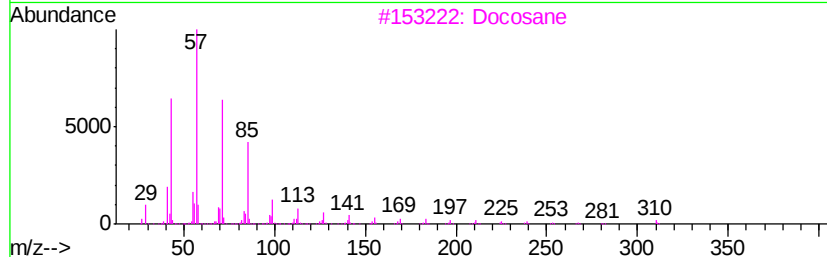
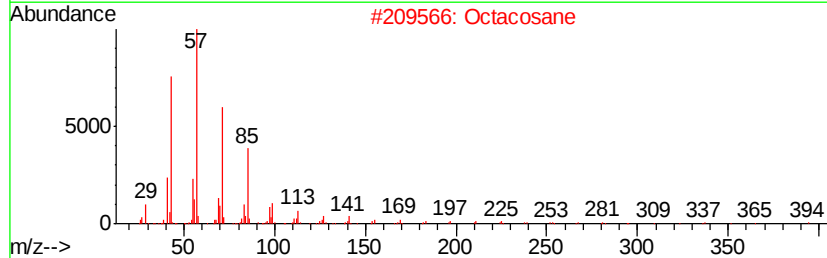
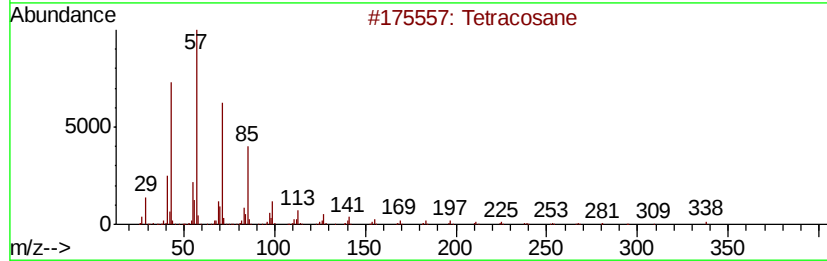
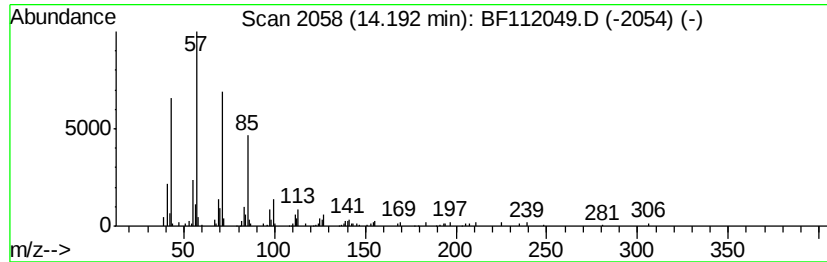
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	3.04 ng	133262	Chrysene-d12	14.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	90
2		Octacosane	394	C28H58	000630-02-4	90
3		Docosane	310	C22H46	000629-97-0	90
4		Hexacosane	366	C26H54	000630-01-3	90
5		Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011419\
Data File : BF112049.D
Acq On : 14 Jan 2019 14:37
Operator : JU/SJ
Sample : K1128-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-200036

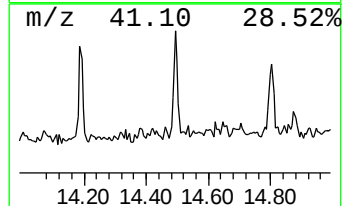
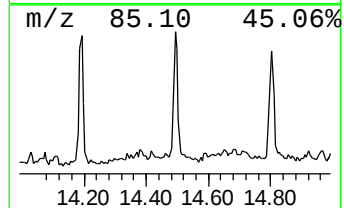
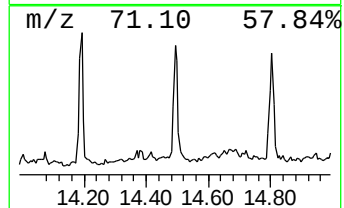
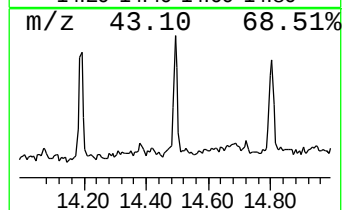
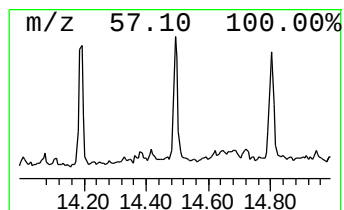
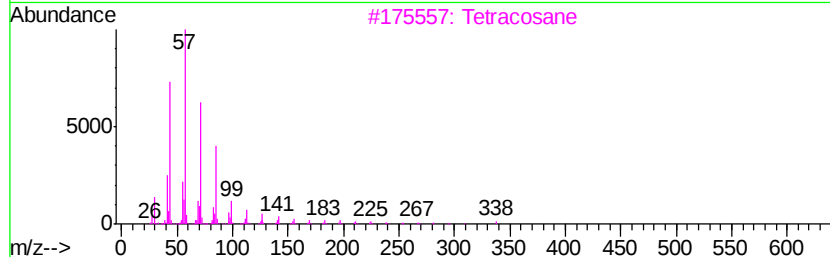
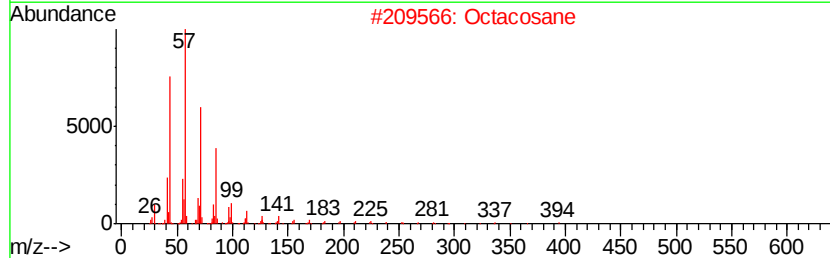
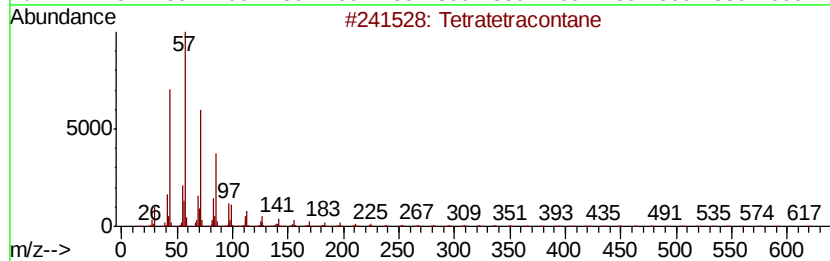
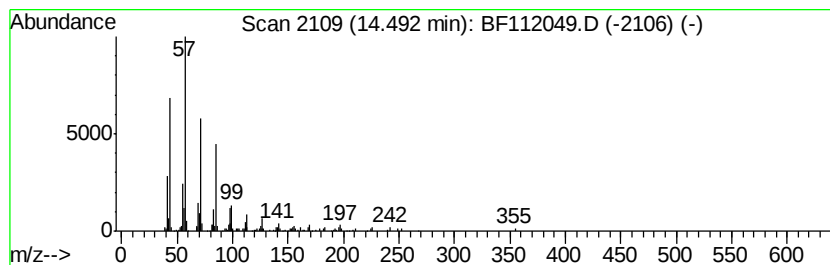
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetratetracontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	2.94 ng	128985	Chrysene-d12	14.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	90
2		Octacosane	394	C28H58	000630-02-4	90
3		Tetracosane	338	C24H50	000646-31-1	90
4		Heptacosane	380	C27H56	000593-49-7	87
5		Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011419\
Data File : BF112049.D
Acq On : 14 Jan 2019 14:37
Operator : JU/SJ
Sample : K1128-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-200036

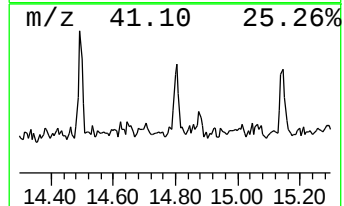
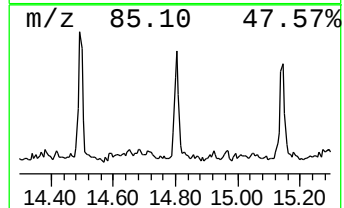
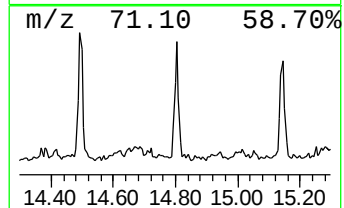
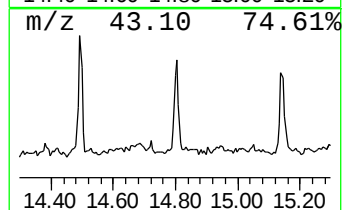
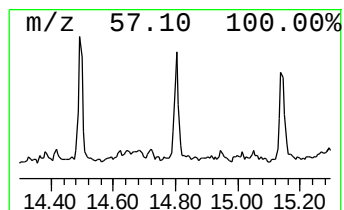
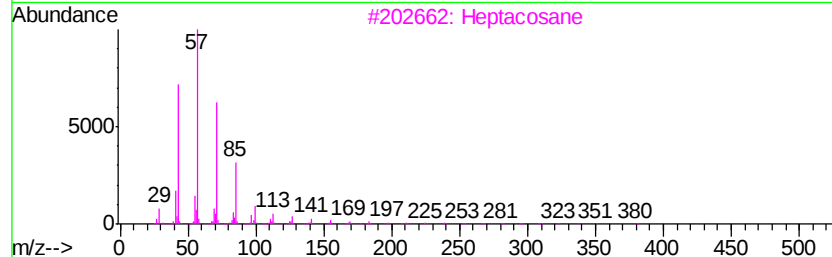
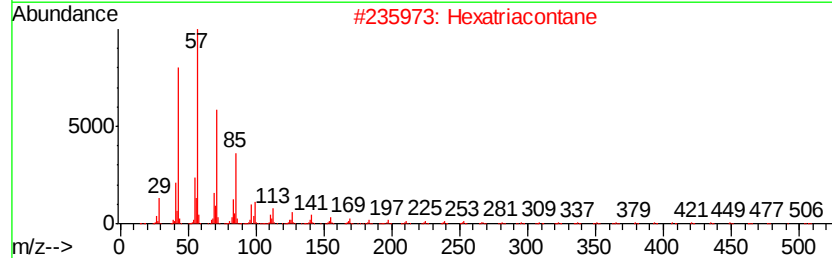
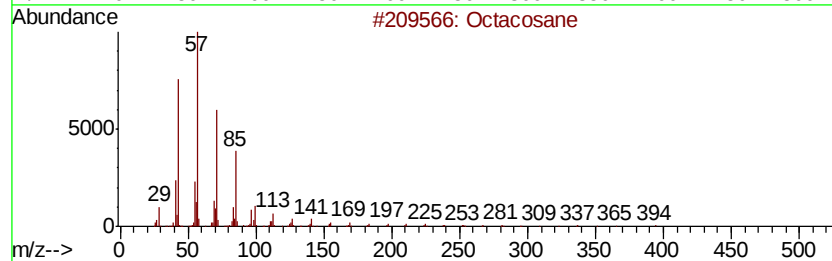
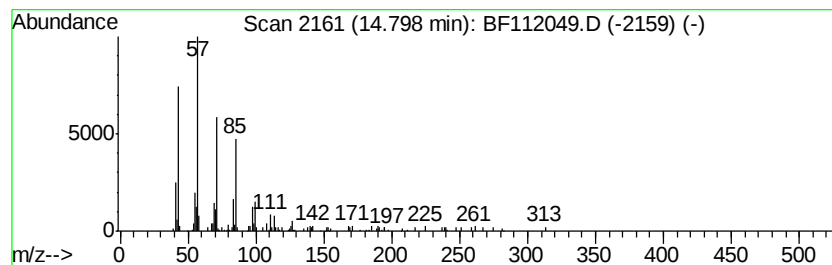
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexatriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	2.49 ng	113781	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	64
2		Hexatriacontane	507	C36H74	000630-06-8	64
3		Heptacosane	380	C27H56	000593-49-7	64
4		Heptadecane, 2-methyl-	254	C18H38	001560-89-0	59
5		Eicosane	282	C20H42	000112-95-8	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011419\
Data File : BF112049.D
Acq On : 14 Jan 2019 14:37
Operator : JU/SJ
Sample : K1128-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-200036

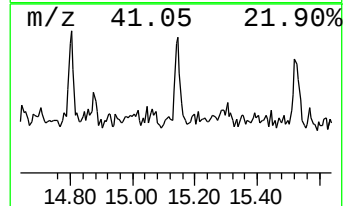
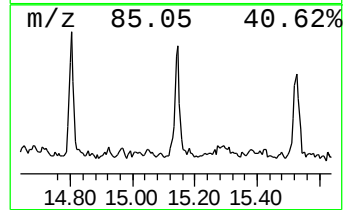
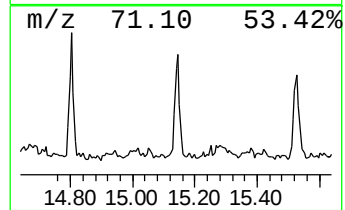
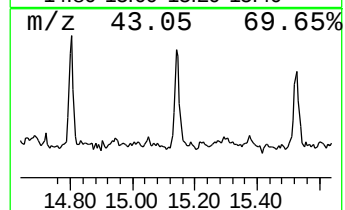
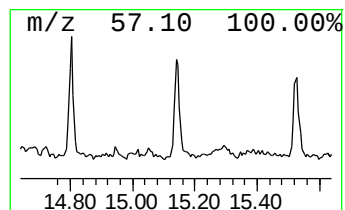
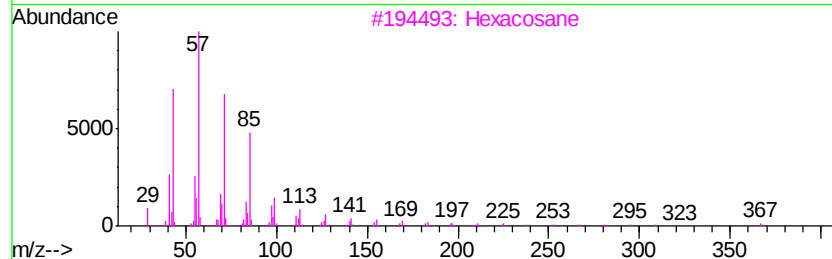
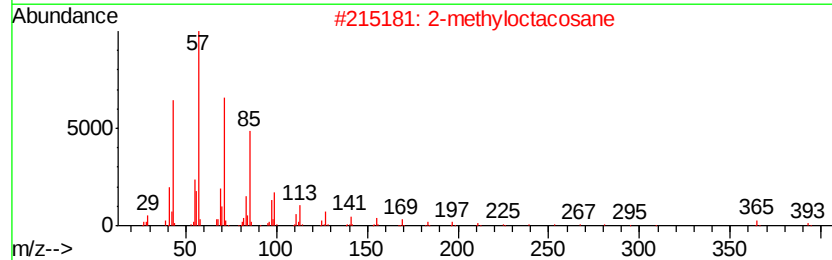
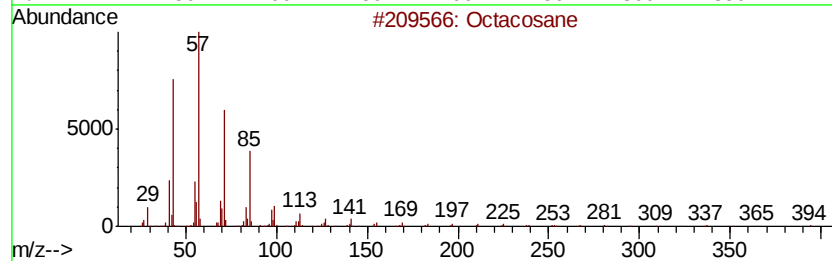
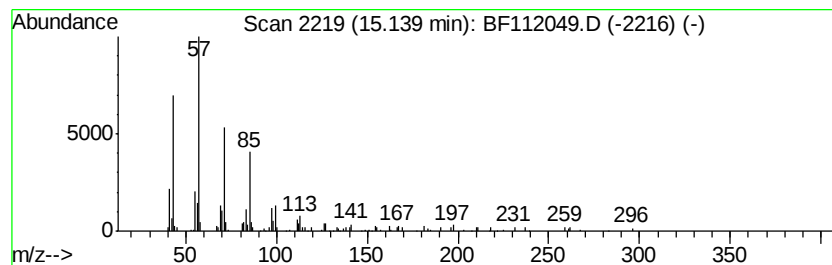
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	2.68 ng	122406	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	90
2		2-methyloctacosane	408	C29H60	1000376-72-8	87
3		Hexacosane	366	C26H54	000630-01-3	86
4		Heptacosane	380	C27H56	000593-49-7	86
5		Heneicosane	296	C21H44	000629-94-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF011419\
Data File : BF112049.D
Acq On : 14 Jan 2019 14:37
Operator : JU/SJ
Sample : K1128-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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...	2.15	3.0	ng	117643	1	6.87	798778	20.0
2-Pentanone, 4-hy...	5.08	3.9	ng	154635	1	6.87	798778	20.0
unknown6.65	6.65	72.8	ng	2905640	1	6.87	798778	20.0
unknown12.85	12.85	2.8	ng	123506	5	14.03	877489	20.0
Sulfurous acid, b...	13.87	4.5	ng	198492	5	14.03	877489	20.0
Tetracosane	14.19	3.0	ng	133262	5	14.03	877489	20.0
Tetratetracontane	14.49	2.9	ng	128985	5	14.03	877489	20.0
Hexatriacontane	14.80	2.5	ng	113781	6	15.51	913790	20.0
Octacosane	15.14	2.7	ng	122406	6	15.51	913790	20.0