

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111518\
 Data File : BF110800.D
 Acq On : 15 Nov 2018 20:40
 Operator : JU/SJ
 Sample : J5942-05
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VW-F1

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-BF110818.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	2.216	18	22	32	rVB	64543	98182	8.51%	0.966%
2	5.169	520	524	533	rBV	24515	37207	3.23%	0.366%
3	5.557	586	590	606	rBV	945608	992165	86.05%	9.764%
4	6.563	757	761	782	rBV	1021272	1084111	94.02%	10.669%
5	6.710	782	786	798	rVV	1179649	1075904	93.31%	10.589%
6	6.939	821	825	832	rBV	339455	298771	25.91%	2.940%
7	7.092	848	851	865	rBV	951511	823340	71.41%	8.103%
8	7.504	917	921	943	rBV	639258	648742	56.26%	6.385%
9	8.222	1040	1043	1067	rBV	365347	381551	33.09%	3.755%
10	9.292	1222	1225	1242	rBV	1195187	1153054	100.00%	11.348%
11	9.692	1290	1293	1301	rBV	81661	76168	6.61%	0.750%
12	9.980	1339	1342	1353	rBV	392064	383899	33.29%	3.778%
13	10.774	1474	1477	1487	rBV	557526	561057	48.66%	5.522%
14	11.480	1593	1597	1604	rBV	330500	328607	28.50%	3.234%
15	11.980	1679	1682	1687	rBV	32167	32047	2.78%	0.315%
16	12.698	1801	1804	1808	rBV	40371	32953	2.86%	0.324%
17	12.933	1837	1844	1849	rVB	43921	50129	4.35%	0.493%
18	13.057	1861	1865	1869	rBV	1045114	920997	79.87%	9.064%
19	13.263	1893	1900	1904	rBV6	8103	14796	1.28%	0.146%
20	13.933	2011	2014	2020	rBV2	61867	74467	6.46%	0.733%
21	14.127	2043	2047	2057	rBV	364865	419884	36.41%	4.132%
22	14.251	2065	2068	2073	rVB4	17627	19931	1.73%	0.196%
23	14.557	2117	2120	2124	rBV	31417	40792	3.54%	0.401%
24	14.874	2170	2174	2179	rBV	39535	40316	3.50%	0.397%
25	14.951	2185	2187	2191	rVB2	17207	21282	1.85%	0.209%
26	15.221	2230	2233	2240	rVB2	52747	75782	6.57%	0.746%
27	15.621	2297	2301	2304	rBV	39674	55044	4.77%	0.542%
28	15.662	2304	2308	2317	rVB	183691	264012	22.90%	2.598%
29	16.068	2373	2377	2384	rVB	41930	72575	6.29%	0.714%
30	16.598	2464	2467	2475	rVB2	29445	49062	4.25%	0.483%
31	17.221	2568	2573	2579	rBV9	13502	34129	2.96%	0.336%

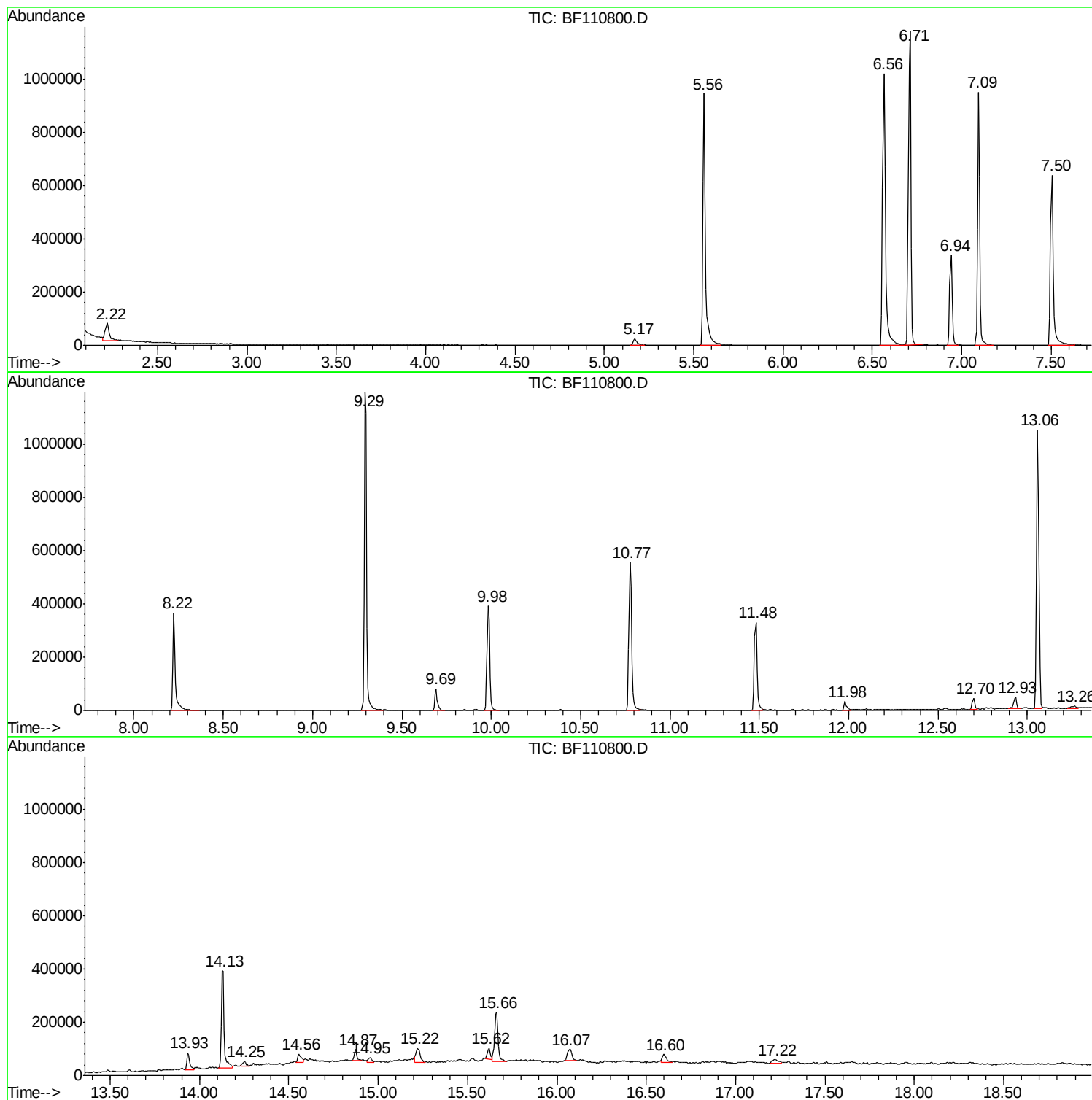
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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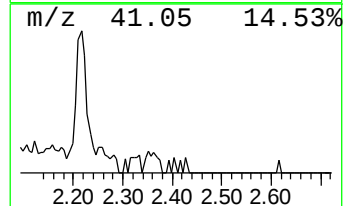
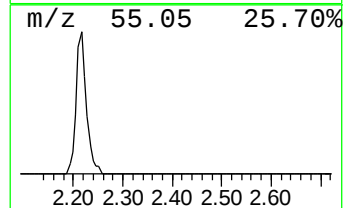
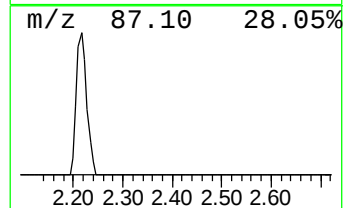
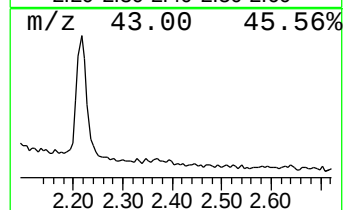
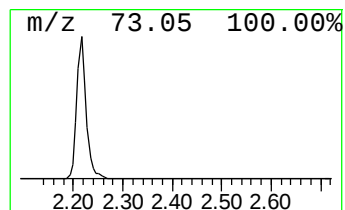
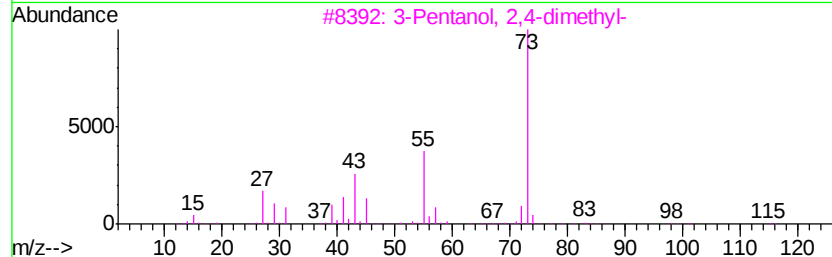
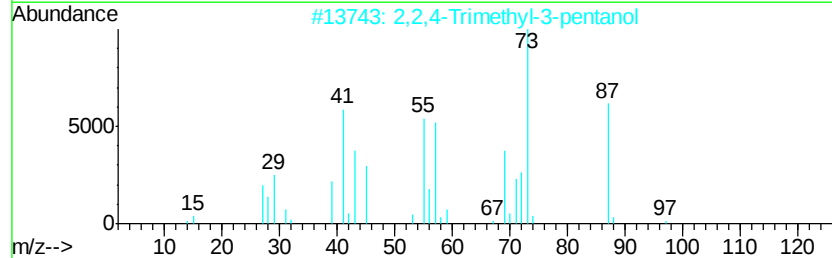
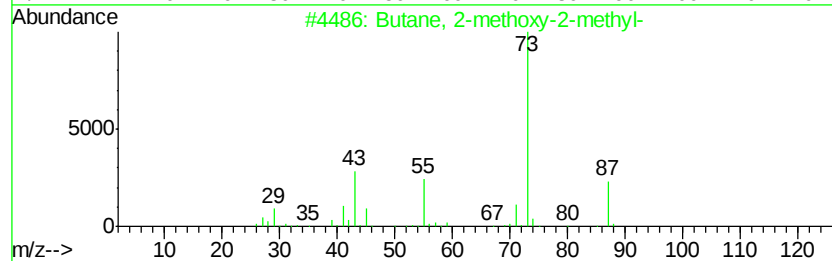
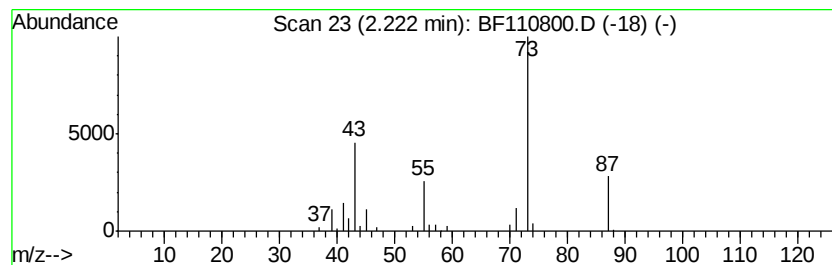
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	6.57 ng	98182	1,4-Dichlorobenzene-d4	6.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	12



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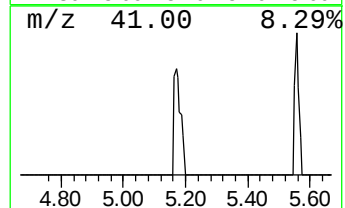
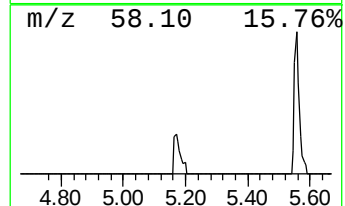
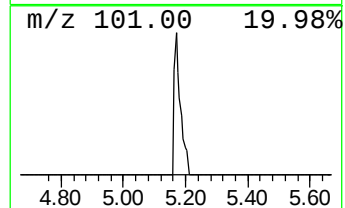
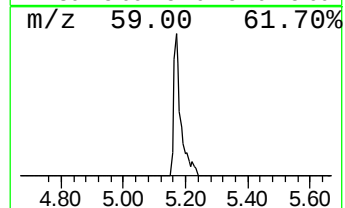
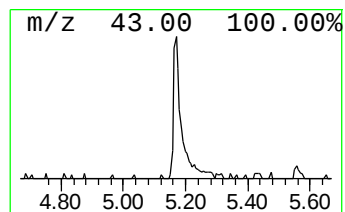
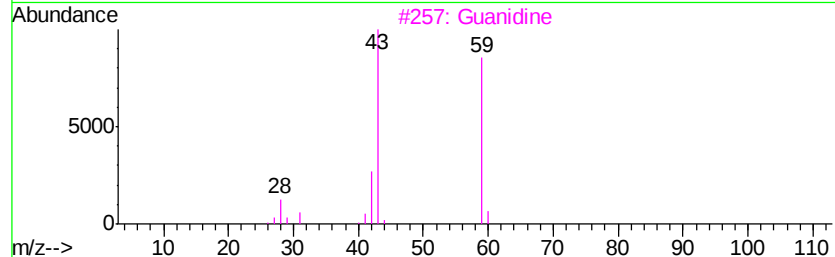
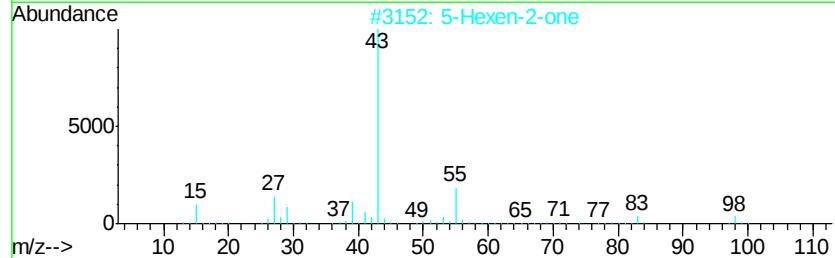
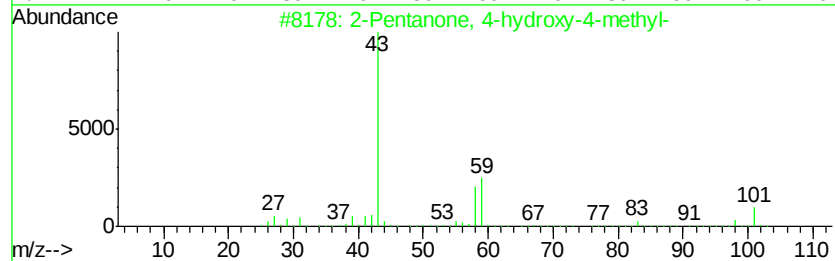
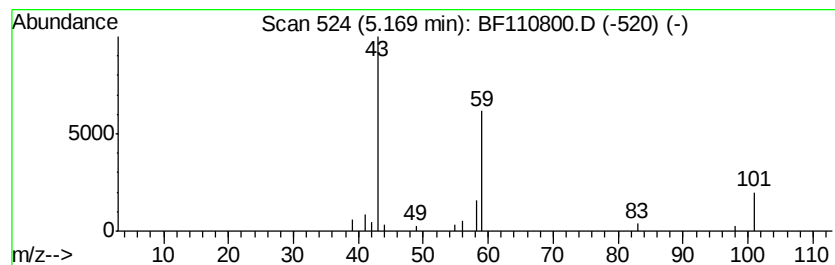
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	2.49 ng	37207	1,4-Dichlorobenzene-d4	6.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2		5-Hexen-2-one	98	C6H10O	000109-49-9	9
3		Guanidine	59	CH5N3	000113-00-8	9
4		3-Hexanol	102	C6H14O	000623-37-0	9
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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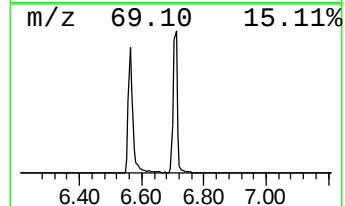
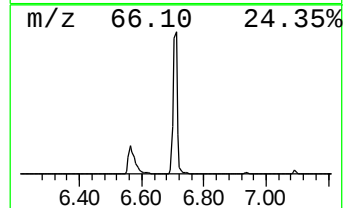
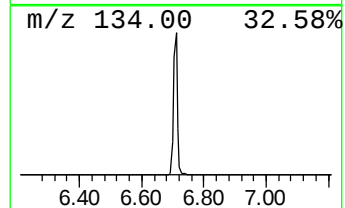
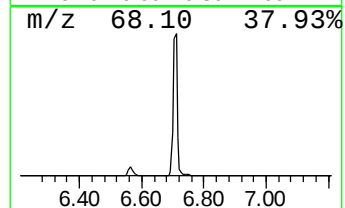
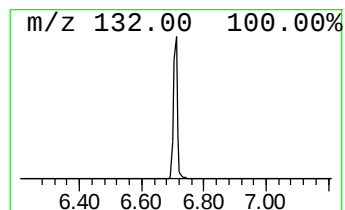
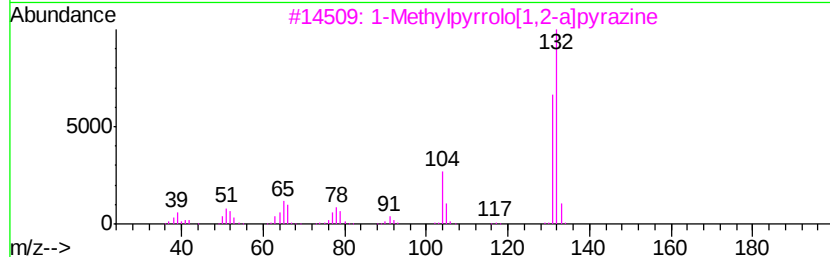
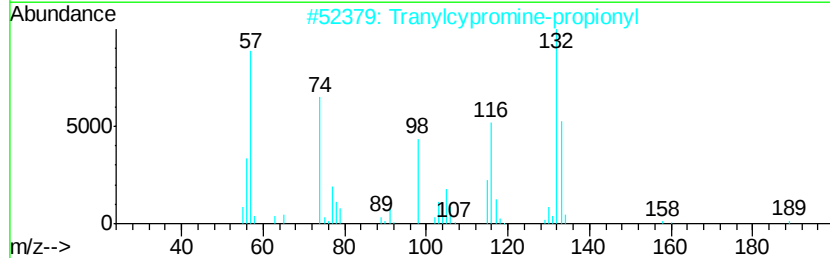
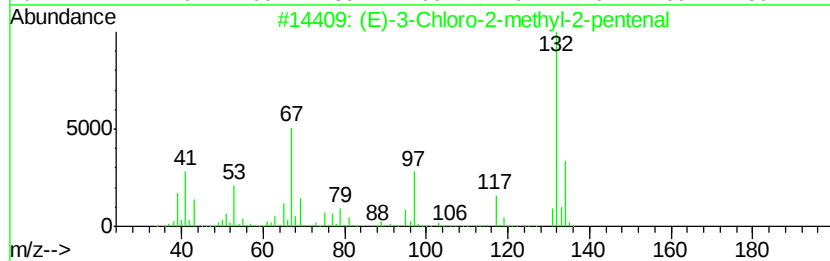
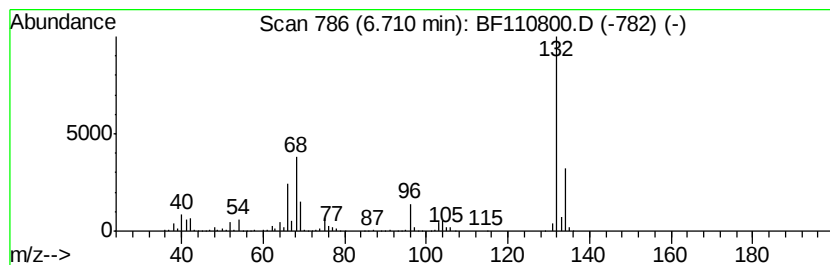
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Peak Number 3 unknown6.71 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	72.02 ng	1075900	1,4-Dichlorobenzene-d4	6.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2		Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9



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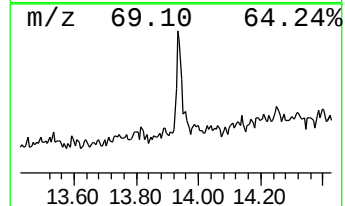
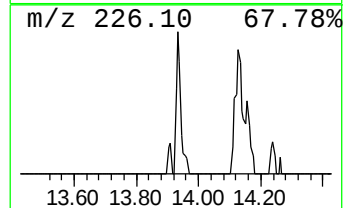
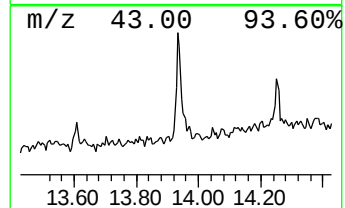
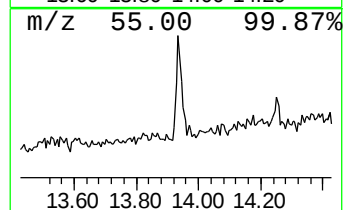
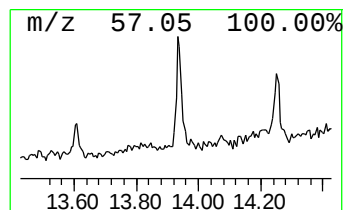
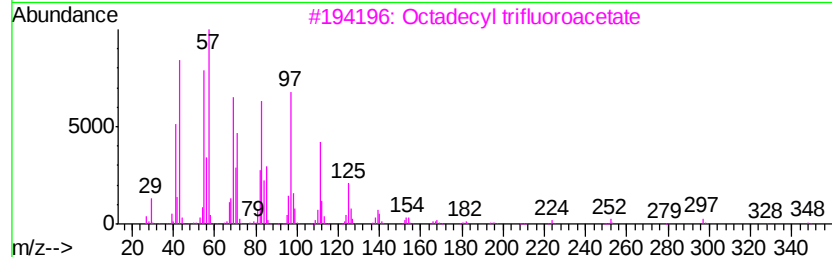
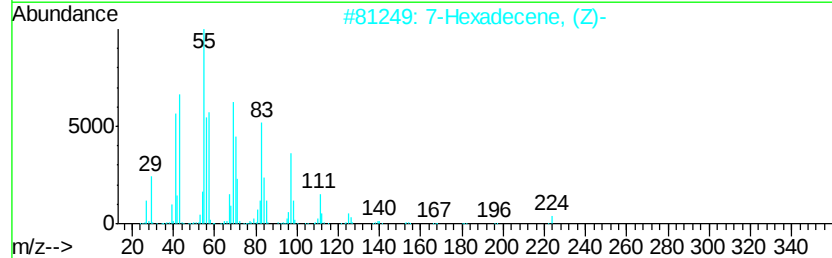
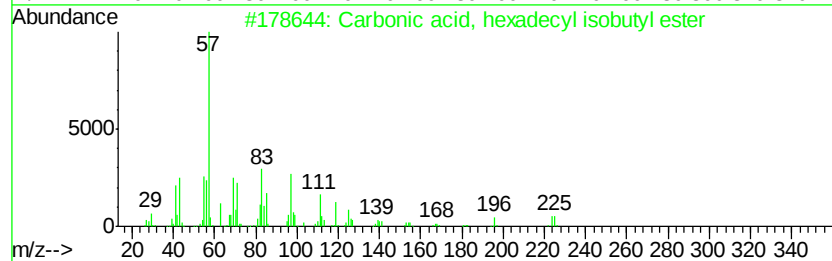
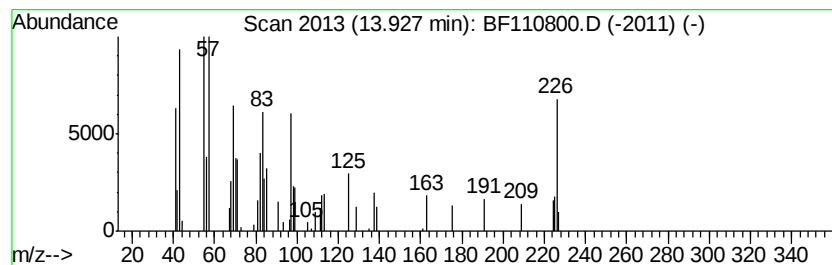
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Peak Number 7 Carbonic acid, hexadecyl is... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	3.55 ng	74467	Chrysene-d12	14.13

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, hexadecyl isobuty...	342	C21H42O3	1000314-61-3	87
2			7-Hexadecene, (Z)-	224	C16H32	035507-09-6	83
3			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	81
4			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	81
5			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	81



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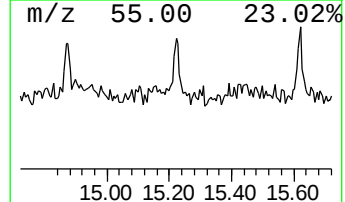
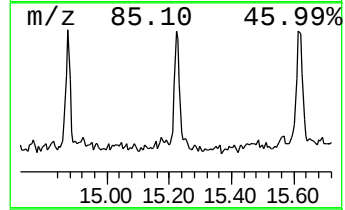
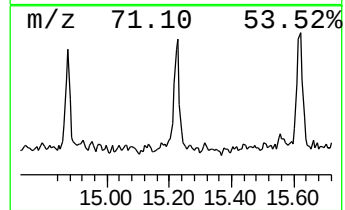
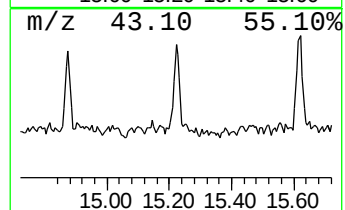
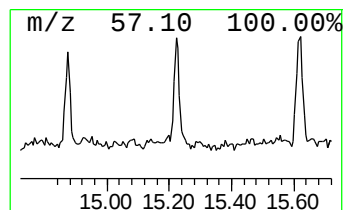
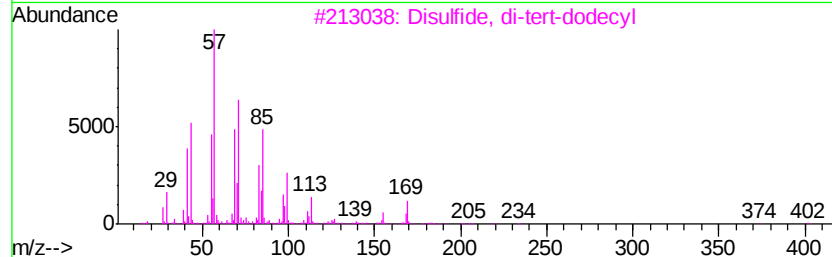
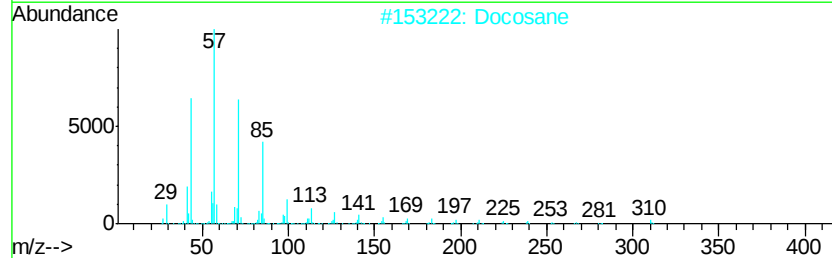
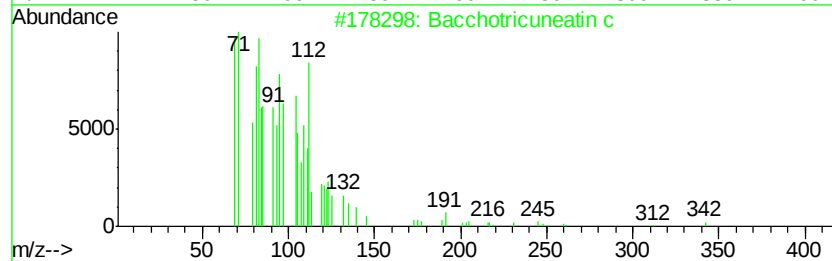
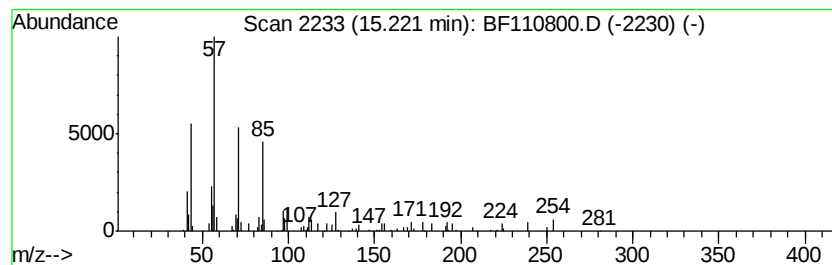
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Peak Number 8 Bacchotricuneatin c Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.22	5.74 ng	75782	Perylene-d12	15.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bacchotricuneatin c	342	C20H22O5	066563-30-2	58
2		Docosane	310	C22H46	000629-97-0	50
3		Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	50
4		Heptacosane	380	C27H56	000593-49-7	50
5		Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	50



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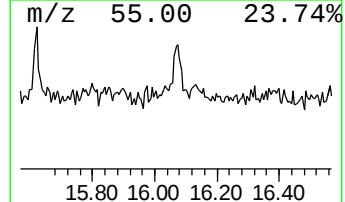
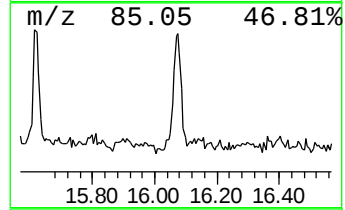
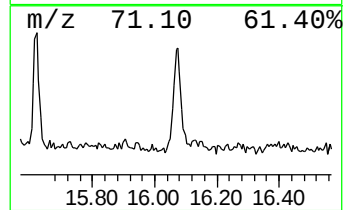
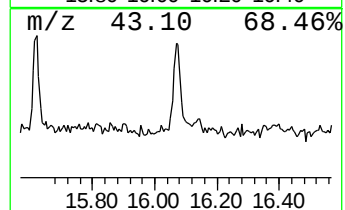
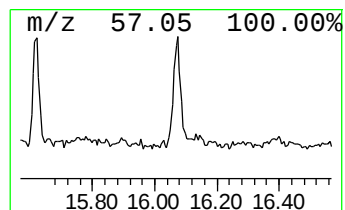
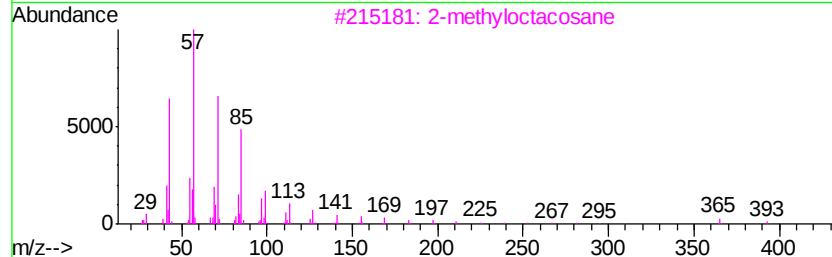
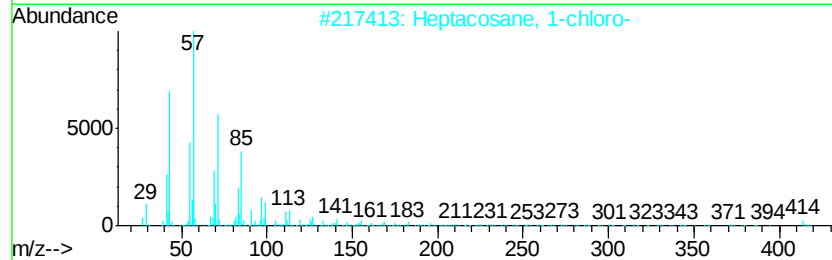
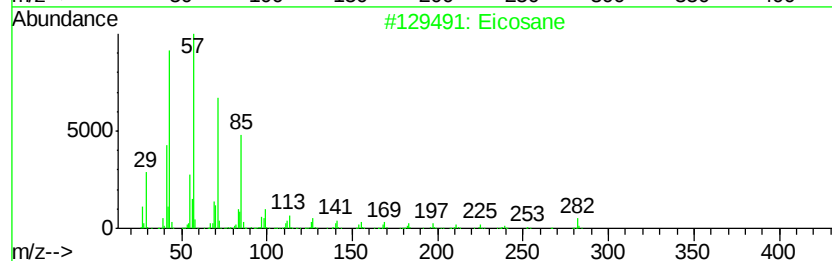
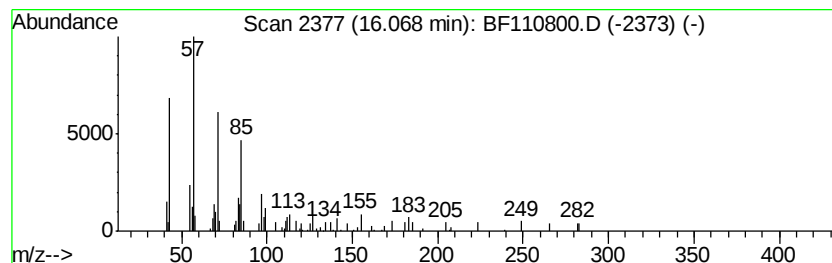
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	5.50 ng	72575	Perylene-d12	15.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	93
2	Heptacosane, 1-chloro-		414	C27H55Cl	062016-79-9	80
3	2-methyloctacosane		408	C29H60	1000376-72-8	80
4	Heptacosane		380	C27H56	000593-49-7	68
5	Octacosane		394	C28H58	000630-02-4	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111518\
Data File : BF110800.D
Acq On : 15 Nov 2018 20:40
Operator : JU/SJ
Sample : J5942-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VW-F1

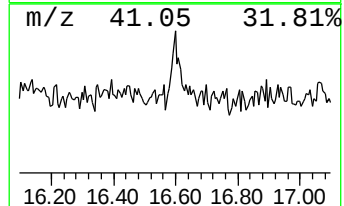
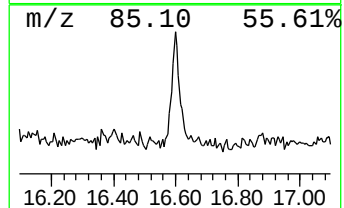
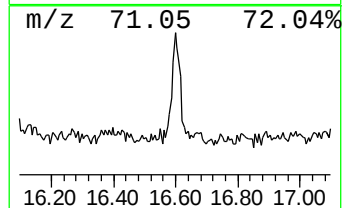
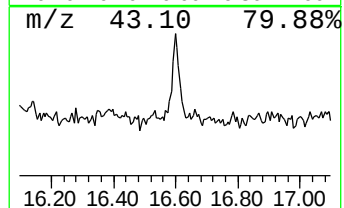
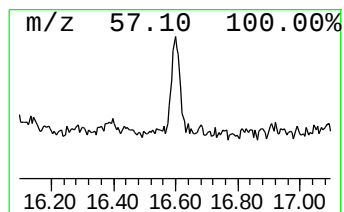
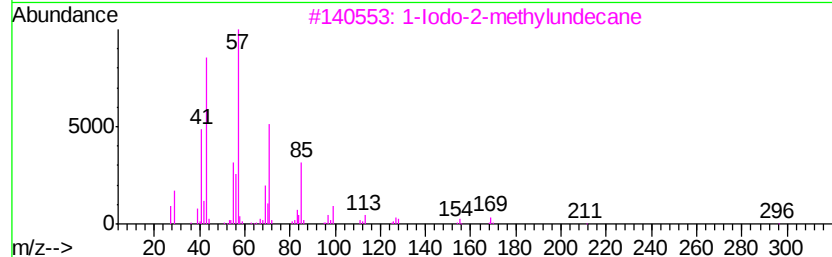
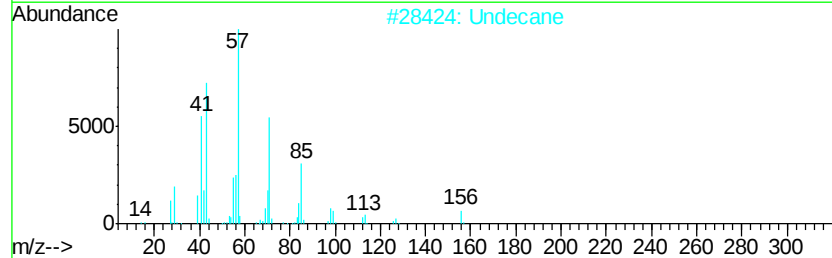
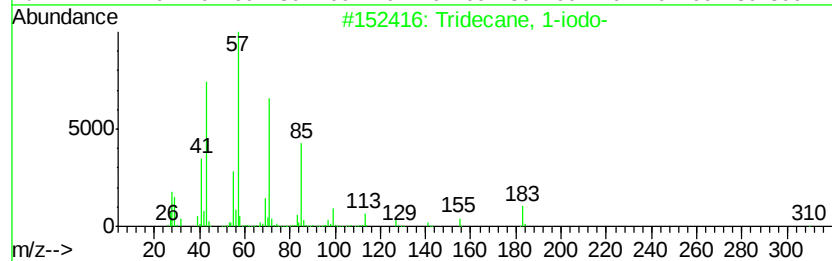
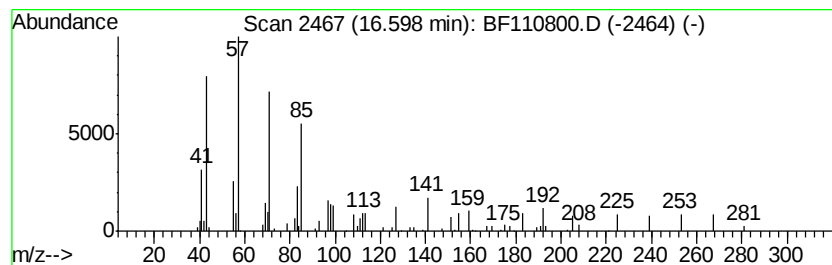
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tridecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.60	3.72 ng	49062	Perylene-d12	15.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	53
2			Undecane	156	C11H24	001120-21-4	53
3			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	50
4			5,5,7,7-Tetraethylundecane	268	C19H40	1000360-42-0	50
5			Dotetracontane	591	C42H86	007098-20-6	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111518\
Data File : BF110800.D
Acq On : 15 Nov 2018 20:40
Operator : JU/SJ
Sample : J5942-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VW-F1

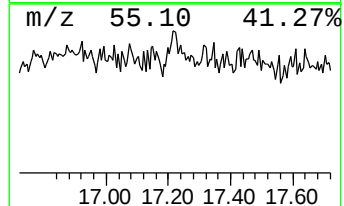
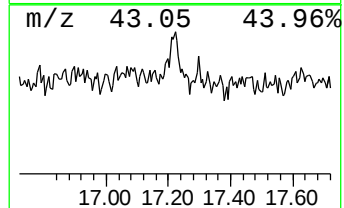
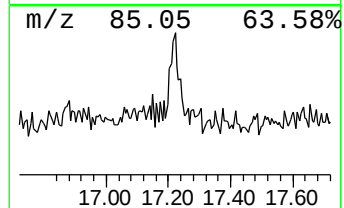
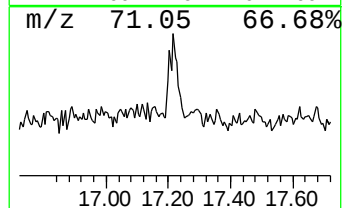
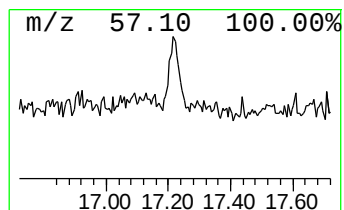
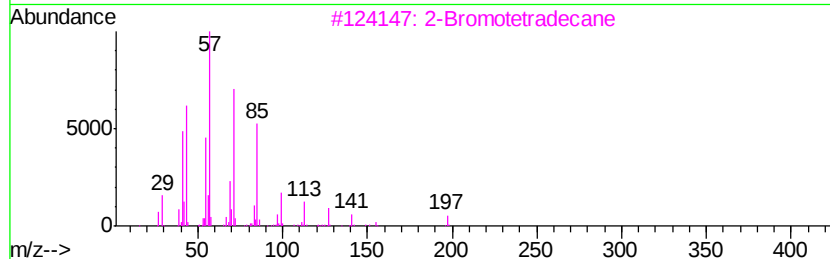
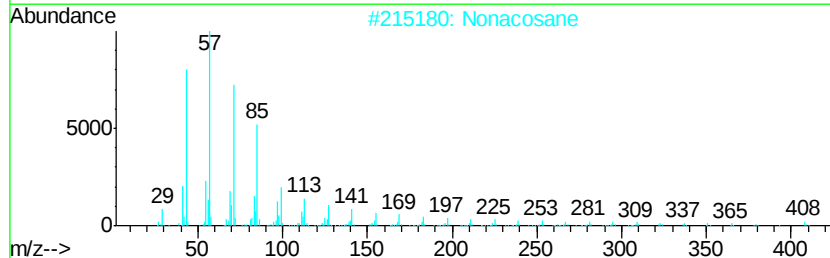
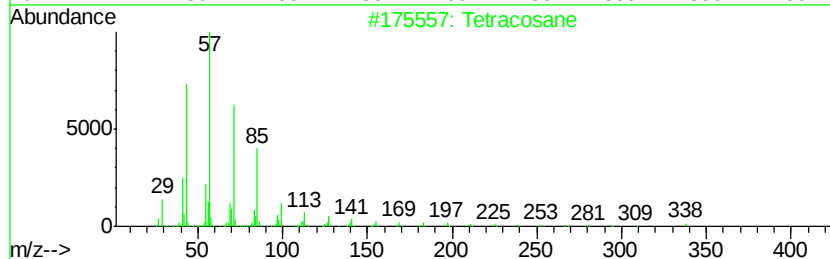
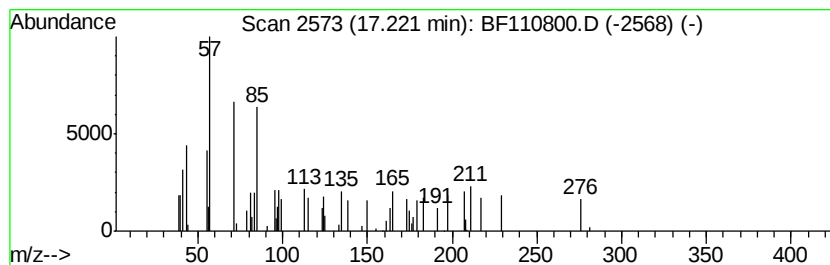
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown17.22 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.22	2.59 ng	34129	Perylene-d12	15.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	27
2		Nonacosane	408	C29H60	000630-03-5	27
3		2-Bromotetradecane	276	C14H29Br	074036-95-6	27
4		Di-n-decylsulfone	346	C20H42O2S	111530-37-1	27
5		Heptadecane	240	C17H36	000629-78-7	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111518\
Data File : BF110800.D
Acq On : 15 Nov 2018 20:40
Operator : JU/SJ
Sample : J5942-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VW-F1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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...	2.22	6.6	ng	98182	1	6.94	298771	20.0
2-Pentanone, 4-hy...	5.17	2.5	ng	37207	1	6.94	298771	20.0
unknown6.71	6.71	72.0	ng	1075900	1	6.94	298771	20.0
Carbonic acid, he...	13.93	3.5	ng	74467	5	14.13	419884	20.0
Bacchotricuneatin c	15.22	5.7	ng	75782	6	15.66	264012	20.0
Eicosane	16.07	5.5	ng	72575	6	15.66	264012	20.0
Tridecane, 1-iodo-	16.60	3.7	ng	49062	6	15.66	264012	20.0
unknown17.22	17.22	2.6	ng	34129	6	15.66	264012	20.0