

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
 Data File : BF111274.D
 Acq On : 11 Dec 2018 13:09
 Operator : JU/SJ
 Sample : J6306-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VB-16204

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-BF120818.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	3.257	197	199	214	rBV	106280	230388	2.01%	0.257%
2	4.657	433	437	440	rBV	125691	138760	1.21%	0.155%
3	5.022	495	499	510	rVB	449995	654641	5.71%	0.730%
4	5.169	515	524	536	rBV	1152763	1373527	11.98%	1.532%
5	5.281	539	543	549	rVB	130629	124319	1.08%	0.139%
6	5.387	556	561	562	rBV2	183107	158712	1.38%	0.177%
7	5.422	562	567	570	rVB	8988219	9676734	84.43%	10.793%
8	5.634	599	603	612	rVB3	177319	246855	2.15%	0.275%
9	6.322	717	720	723	rBV	190010	169632	1.48%	0.189%
10	6.434	731	739	745	rBV2	8842447	11461505	100.00%	12.784%
11	6.487	745	748	757	rVB	165719	158726	1.38%	0.177%
12	6.569	757	762	765	rBV	9722338	10210803	89.09%	11.389%
13	6.628	769	772	777	rVB	348512	287391	2.51%	0.321%
14	6.798	797	801	804	rBV	2427335	2252960	19.66%	2.513%
15	6.957	823	828	831	rBV	7941746	7544005	65.82%	8.414%
16	7.122	853	856	863	rBV2	99698	149648	1.31%	0.167%
17	7.357	890	896	899	rBV	6540887	7092093	61.88%	7.910%
18	7.951	994	997	1000	rVB	211536	169466	1.48%	0.189%
19	8.022	1006	1009	1014	rVB2	72974	117695	1.03%	0.131%
20	8.075	1014	1018	1022	rBV	3324705	3152175	27.50%	3.516%
21	9.157	1196	1202	1205	rBV	10625511	9829704	85.76%	10.964%
22	9.545	1265	1268	1271	rBV	1568939	1181842	10.31%	1.318%
23	9.833	1311	1317	1321	rBV	3897327	3311006	28.89%	3.693%
24	10.622	1446	1451	1454	rBV	6379174	5964140	52.04%	6.652%
25	11.316	1565	1569	1572	rBV	3074634	2603707	22.72%	2.904%
26	11.851	1655	1660	1669	rVB2	1133549	1194523	10.42%	1.332%
27	12.521	1772	1774	1777	rBV	148396	159809	1.39%	0.178%
28	12.633	1790	1793	1799	rBV	451944	423364	3.69%	0.472%
29	12.904	1835	1839	1842	rBV	6206725	5660665	49.39%	6.314%
30	13.363	1911	1917	1919	rBV5	93848	183067	1.60%	0.204%
31	13.810	1990	1993	2002	rVB4	223567	403714	3.52%	0.450%
32	13.951	2013	2017	2020	rBV	1883961	1729625	15.09%	1.929%
33	14.592	2123	2126	2131	rBV2	128604	138058	1.20%	0.154%
34	14.810	2161	2163	2169	rVB	146038	160869	1.40%	0.179%

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.392	2257	2262	2267	rBV	1110654	1343395	11.72%	1.498%
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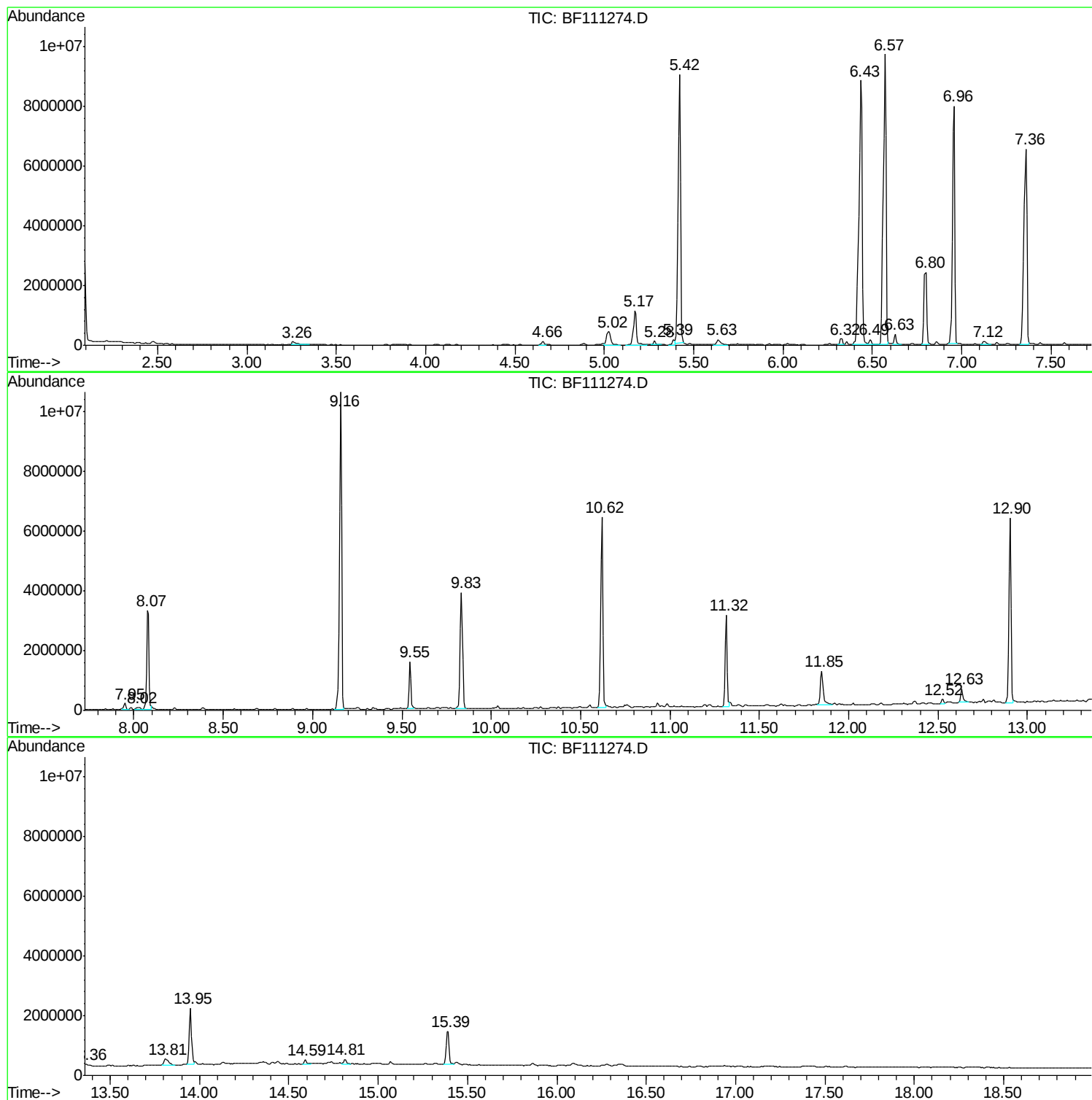
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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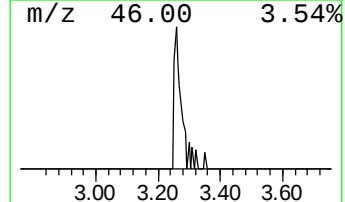
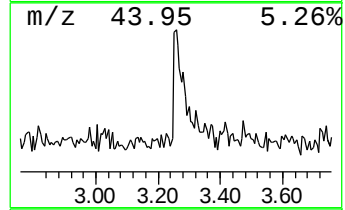
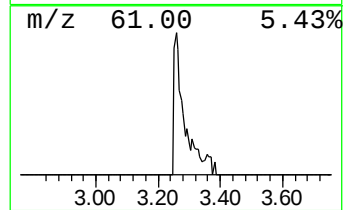
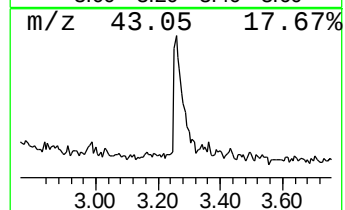
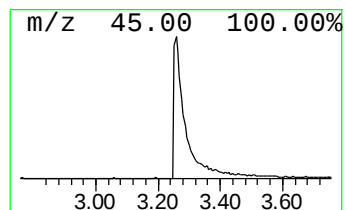
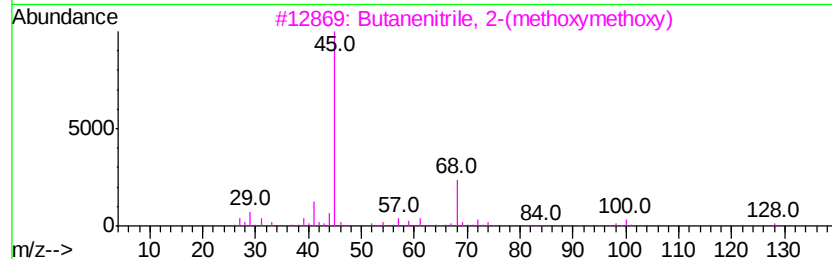
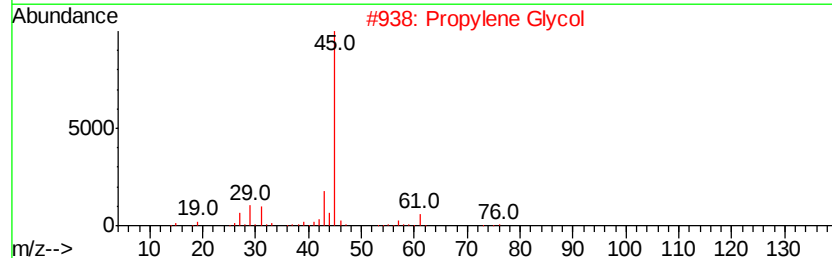
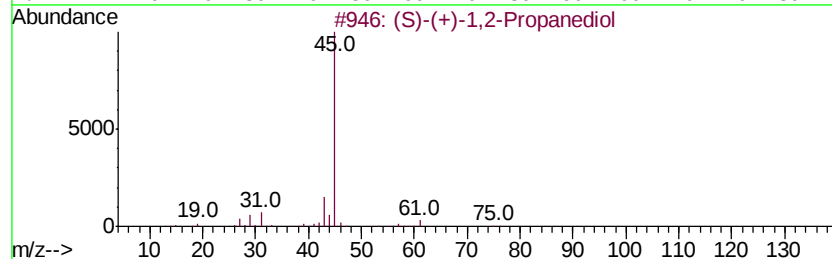
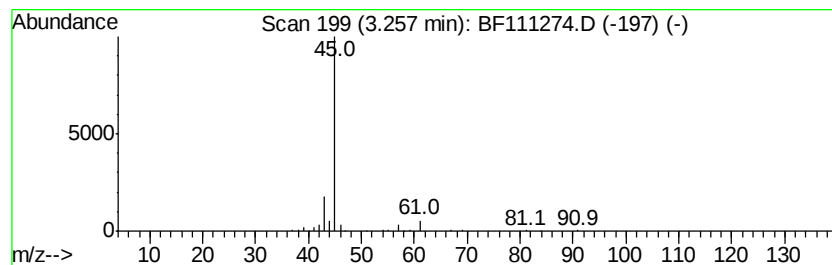
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.26	2.05 ng	230388	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2			Propylene Glycol	76	C3H8O2	000057-55-6	43
3			Butanenitrile, 2-(methoxymethoxy)	129	C6H11NO2	1000196-86-5	9
4			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9



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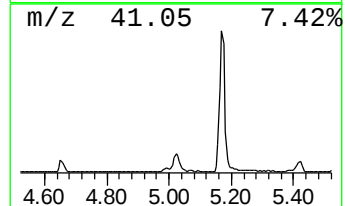
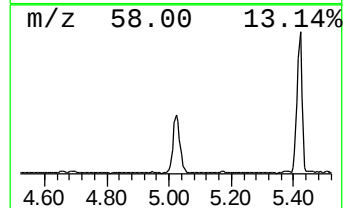
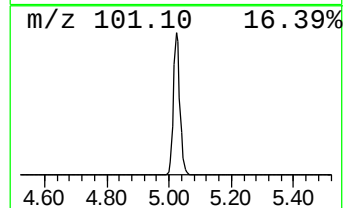
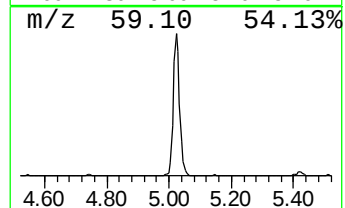
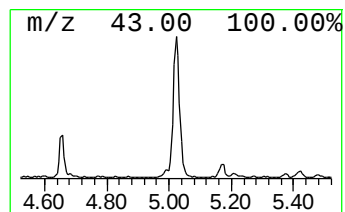
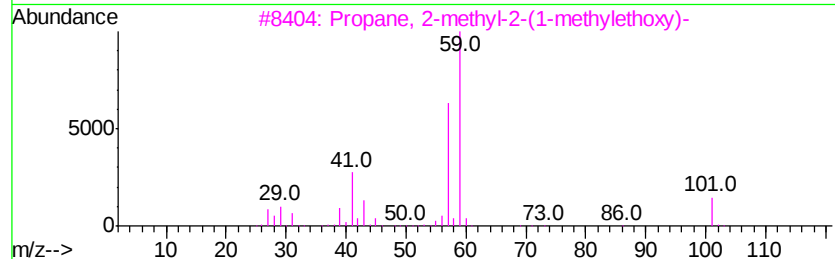
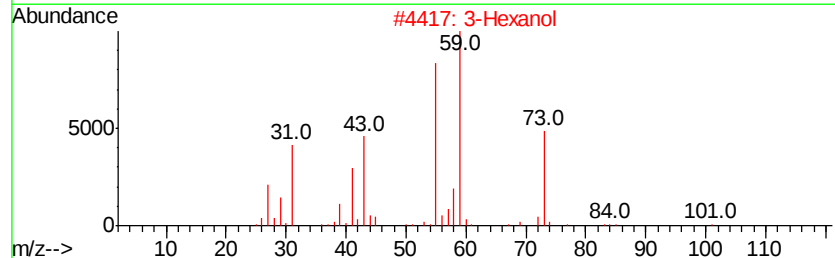
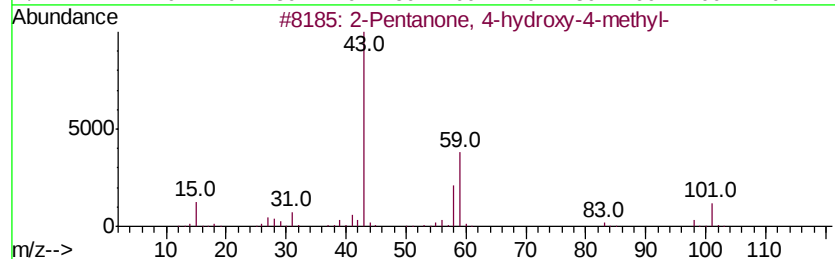
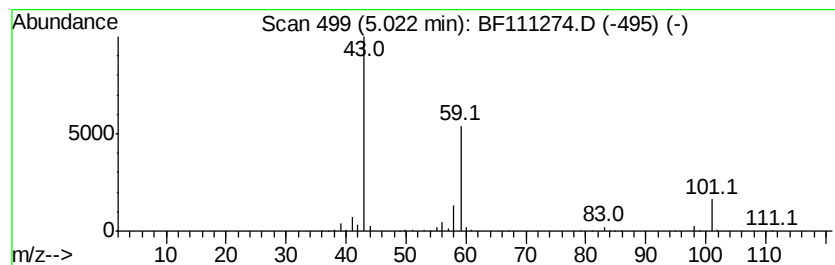
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.02	5.81 ng	654641	1,4-Dichlorobenzene-d4	6.80	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol	102	C6H14O	000623-37-0	33
3	Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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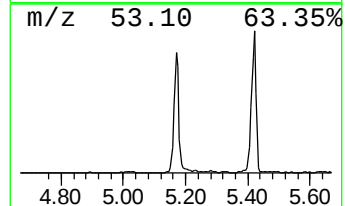
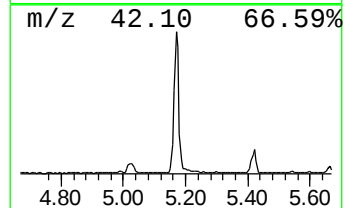
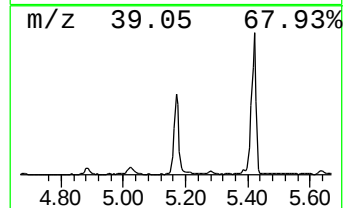
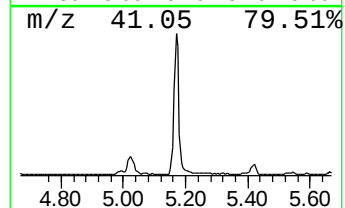
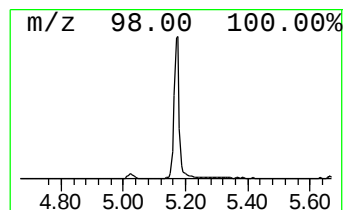
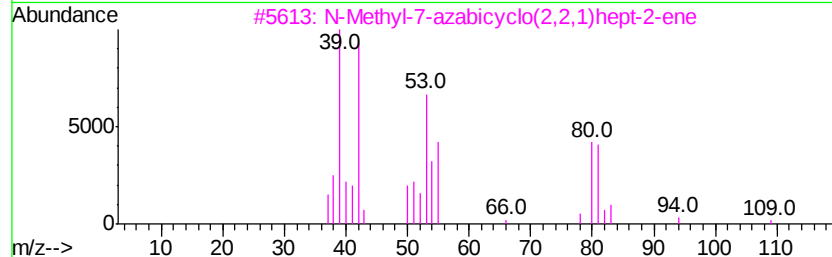
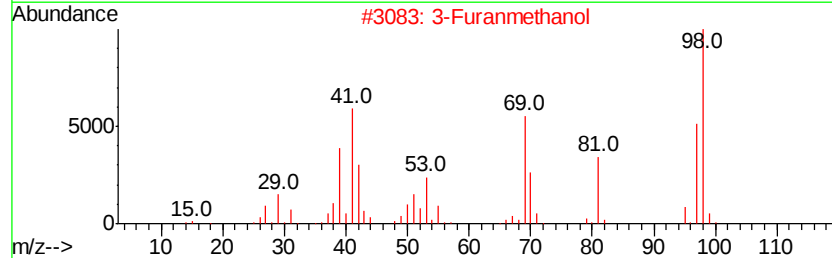
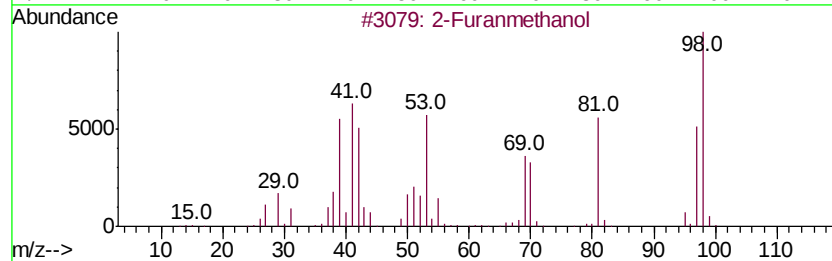
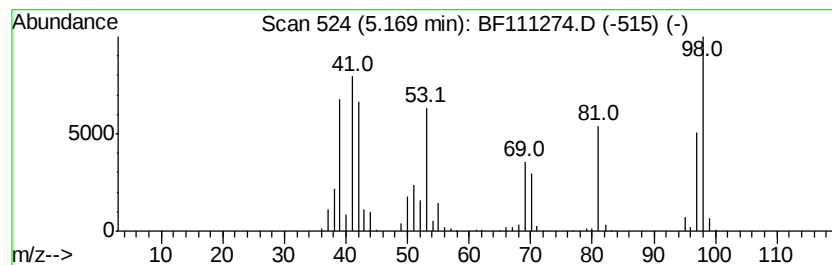
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Furanmethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	12.19 ng	1373530	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Furanmethanol	98	C5H6O2	000098-00-0	98
2		3-Furanmethanol	98	C5H6O2	004412-91-3	70
3		N-Methyl-7-azabicyclo(2.2.1)hept...	109	C7H11N	055590-26-6	42
4		Methylenecyclopropanecarboxylic ...	98	C5H6O2	062266-36-8	38
5		Thiocyanic acid, 2-propynyl ester	97	C4H3NS	024309-48-6	30



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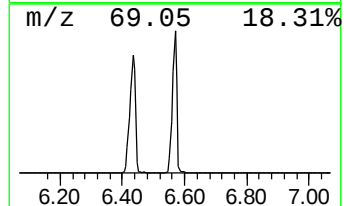
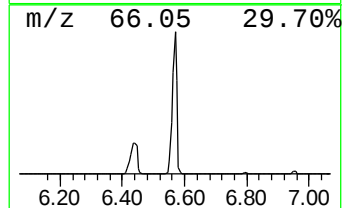
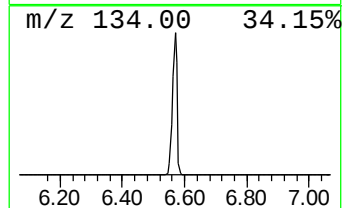
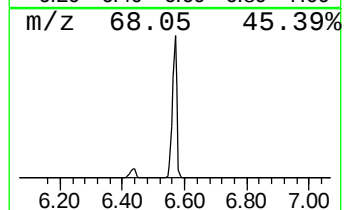
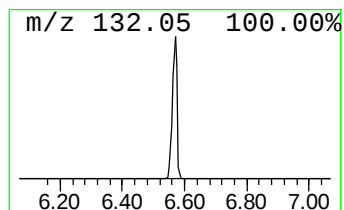
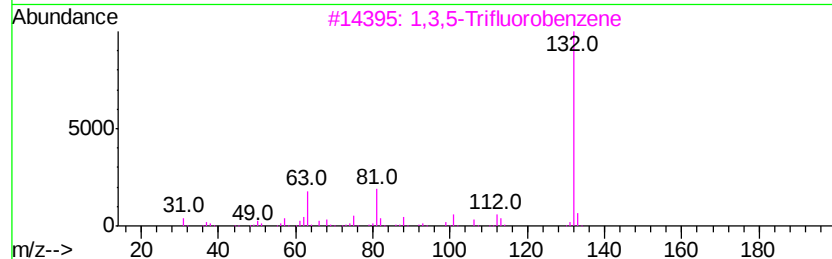
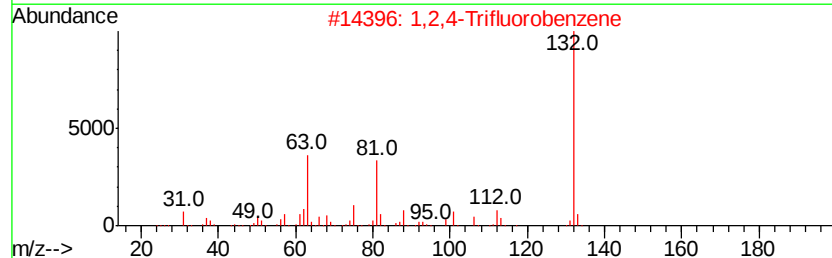
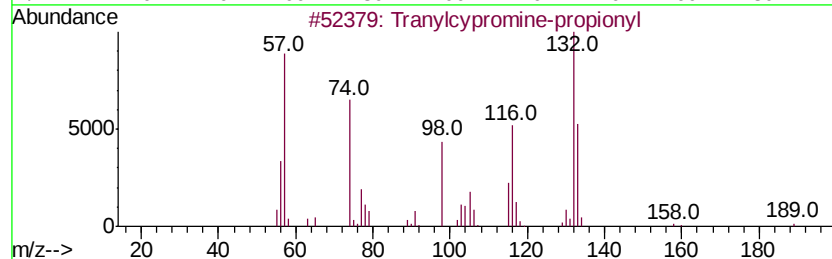
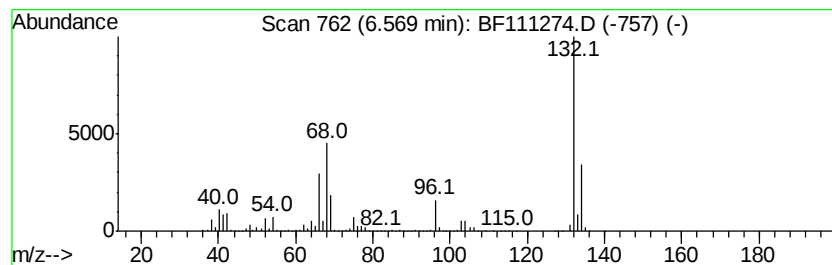
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	90.64 ng	10210800	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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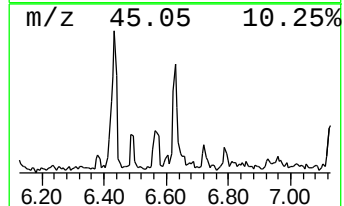
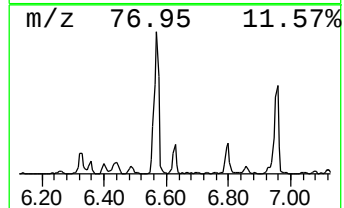
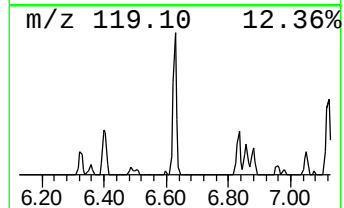
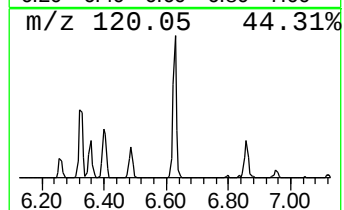
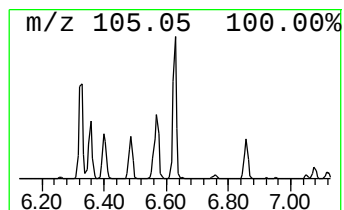
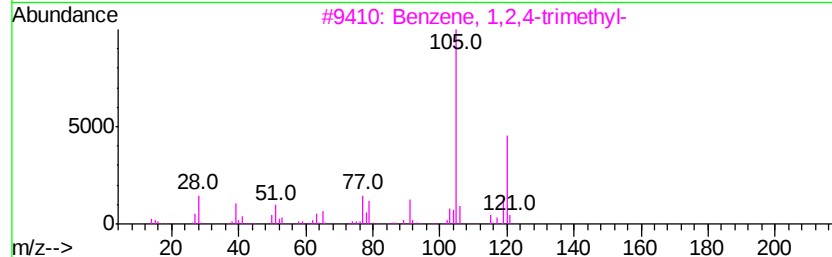
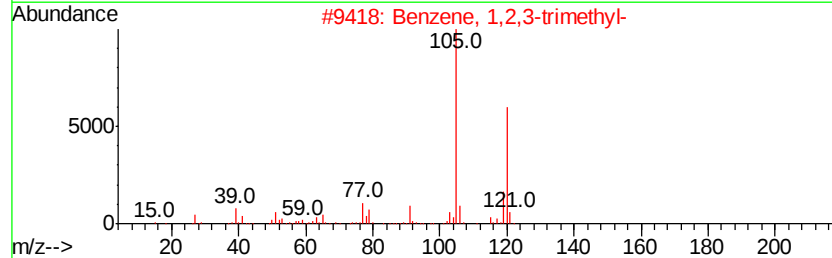
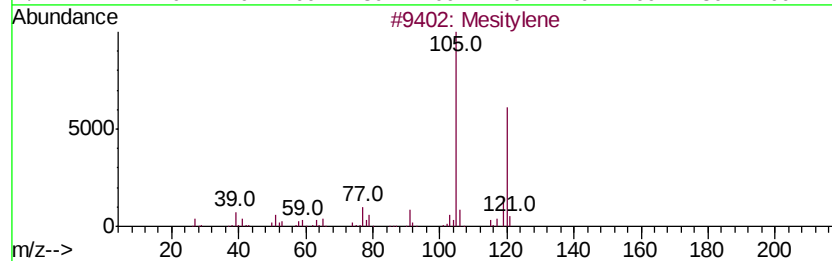
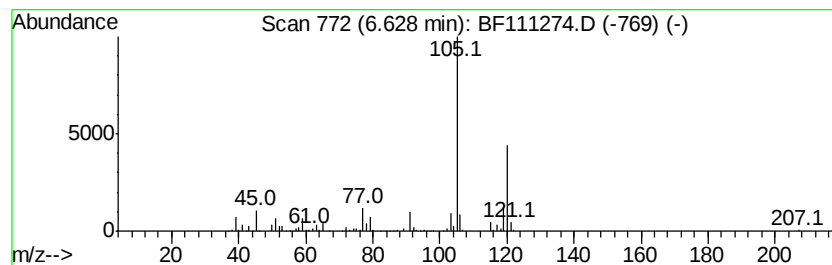
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Mesitylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	2.55 ng	287391	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Mesitylene	120	C9H12	000108-67-8	95
2		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	87
5		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111274.D
Acq On : 11 Dec 2018 13:09
Operator : JU/SJ
Sample : J6306-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

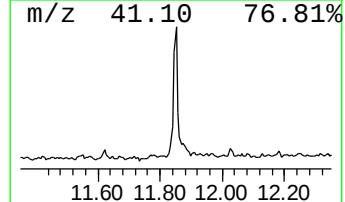
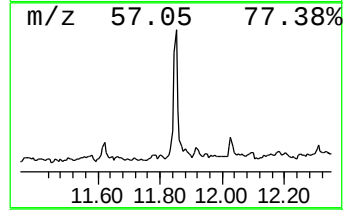
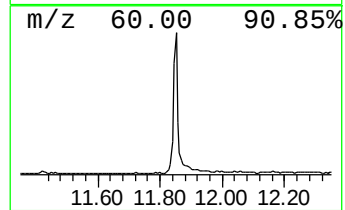
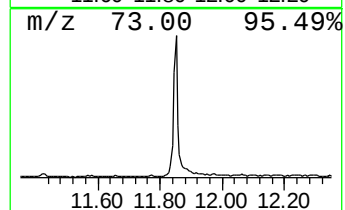
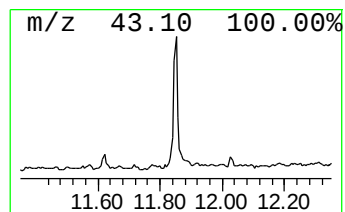
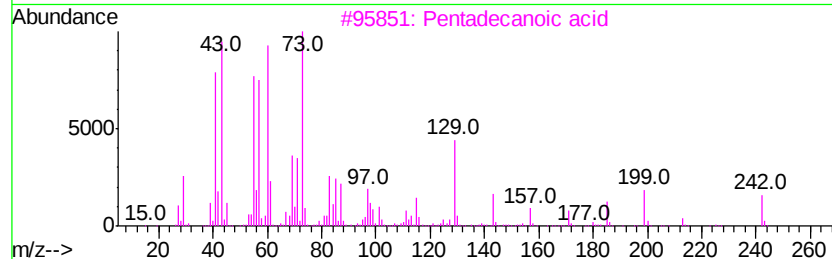
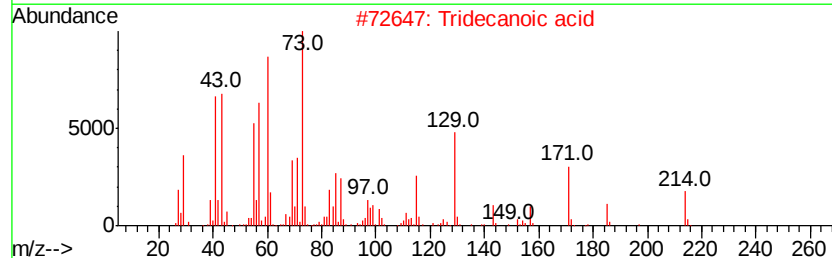
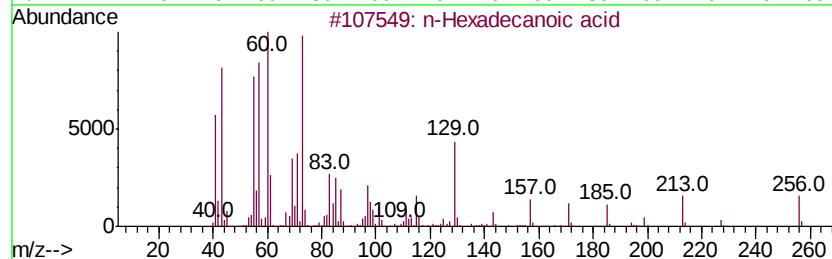
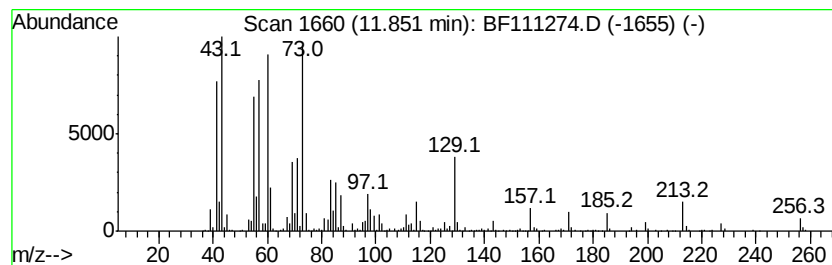
Instrument :
BNA_F
ClientSampleId :
VB-16204

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.85	9.18 ng	1194520	Phenanthrene-d10		11.32	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	90
5	n-Decanoic acid		172	C10H20O2	000334-48-5	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111274.D
Acq On : 11 Dec 2018 13:09
Operator : JU/SJ
Sample : J6306-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

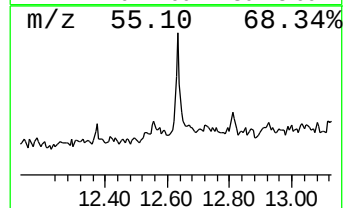
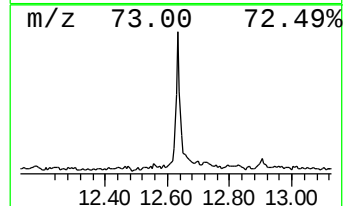
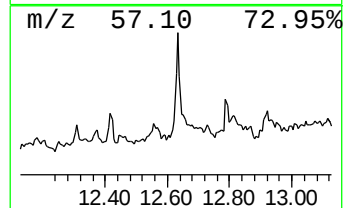
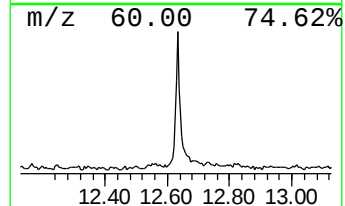
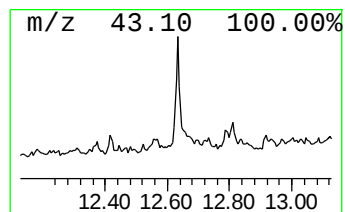
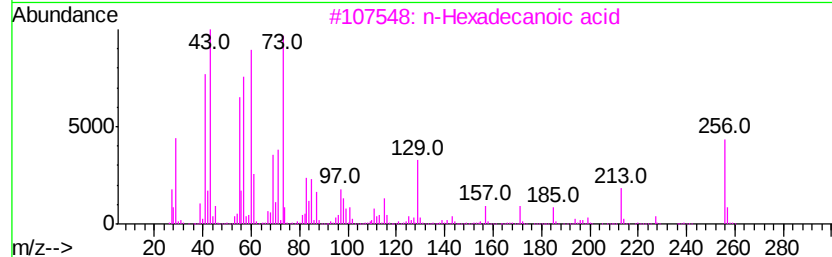
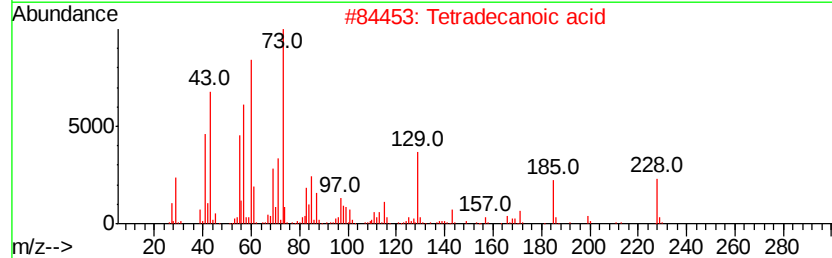
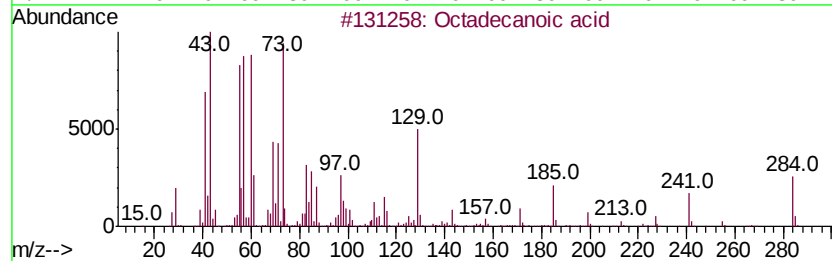
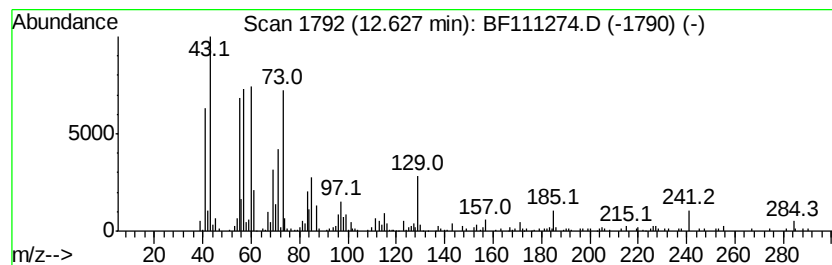
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ClientSampleId :
VB-16204

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.63	3.25 ng	423364	Phenanthrene-d10		11.32
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111274.D
Acq On : 11 Dec 2018 13:09
Operator : JU/SJ
Sample : J6306-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VB-16204

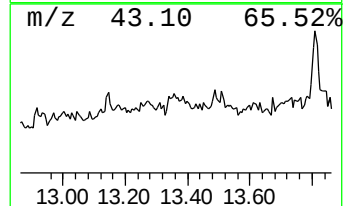
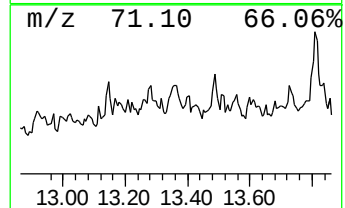
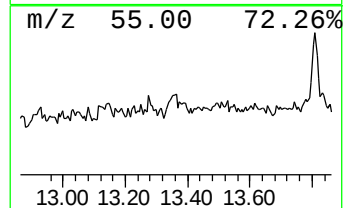
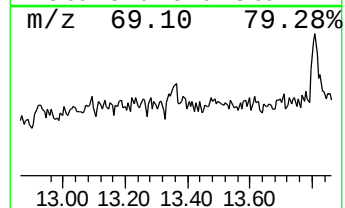
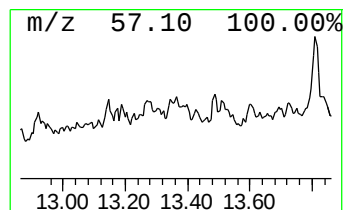
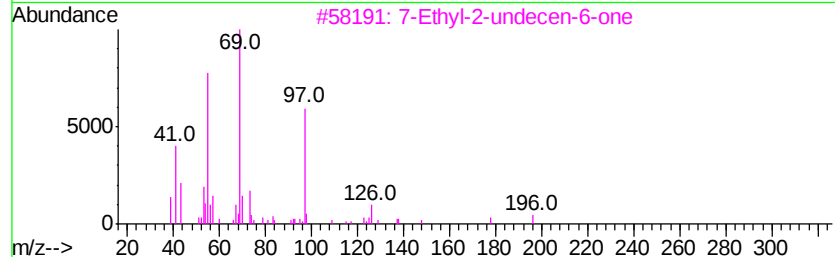
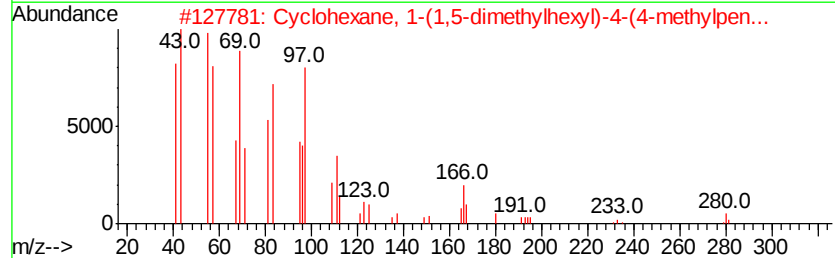
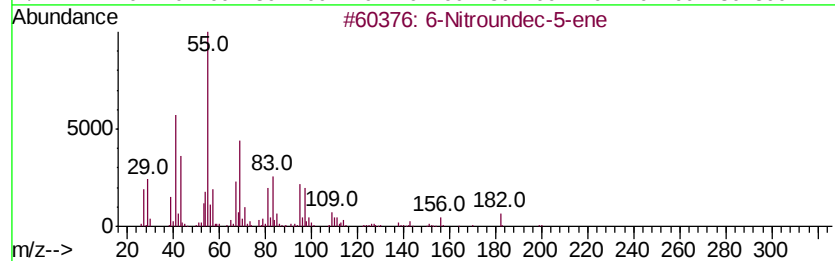
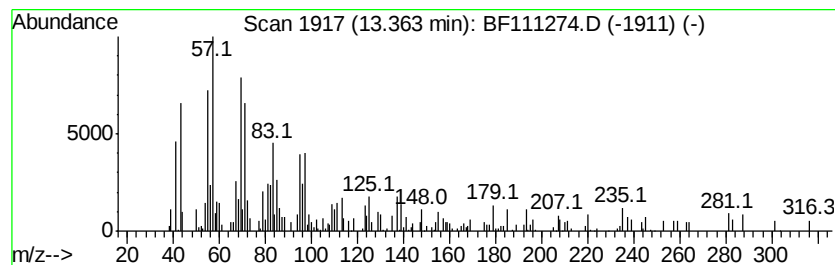
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown13.36 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	2.12 ng	183067	Chrysene-d12	13.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6-Nitroundec-5-ene	199	C11H21NO2	1000192-40-3	38
2			Cyclohexane, 1-(1,5-dimethylhexyl)-4-(4-methylpen...	280	C20H40	056009-20-2	38
3			7-Ethyl-2-undecen-6-one	196	C13H24O	1000374-14-9	30
4			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	30
5			Pentanoic acid, 4-methyl-4-nitro...	175	C7H13NO4	016507-02-1	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
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Sample : J6306-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VB-16204

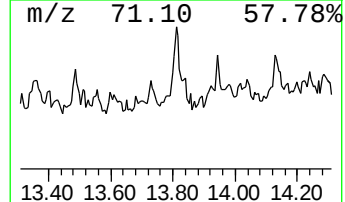
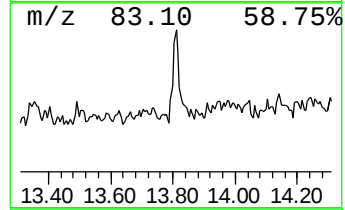
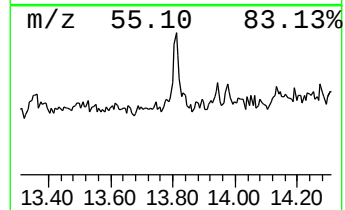
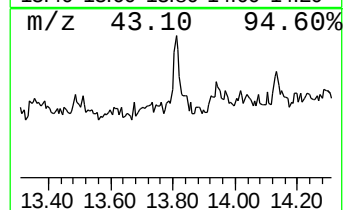
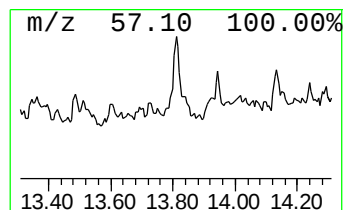
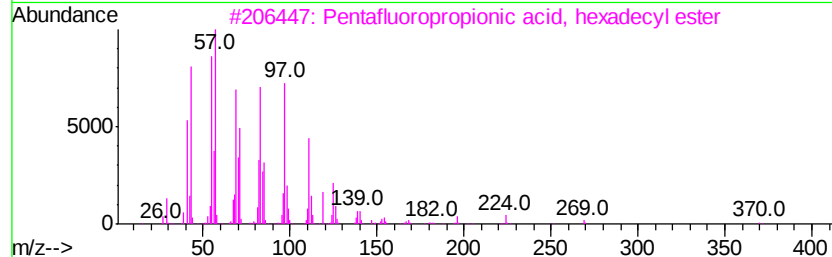
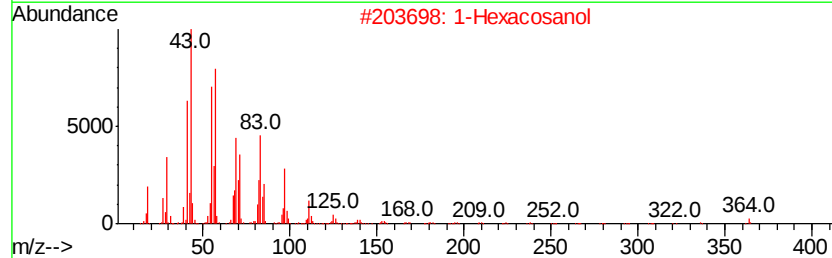
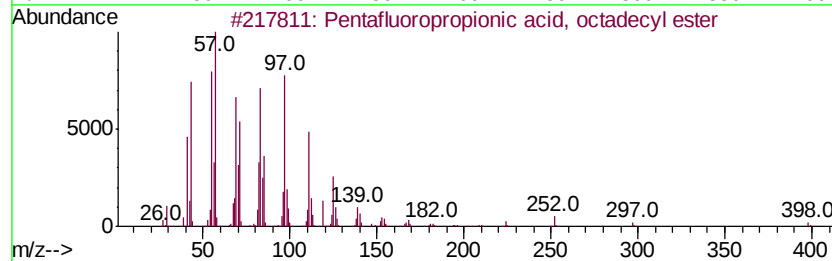
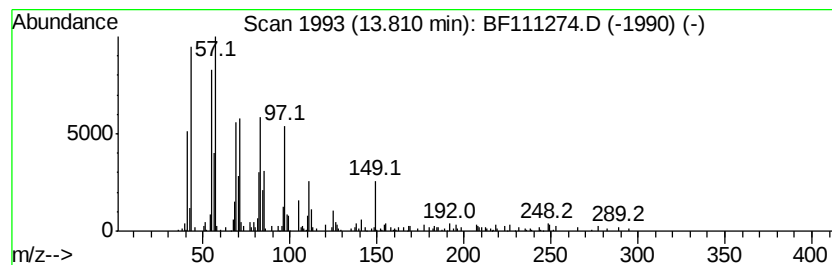
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	4.67 ng	403714	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	83
2		1-Hexacosanol	382	C26H54O	000506-52-5	83
3		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	83
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	83
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111274.D
Acq On : 11 Dec 2018 13:09
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Sample : J6306-01
Misc :
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Instrument :
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ClientSampleId :
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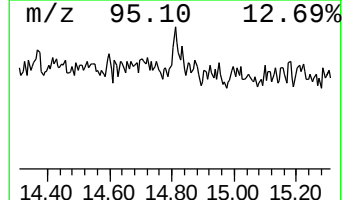
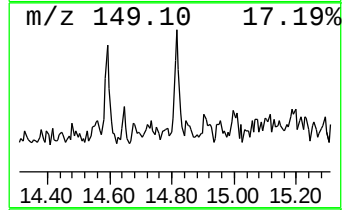
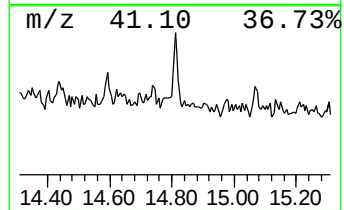
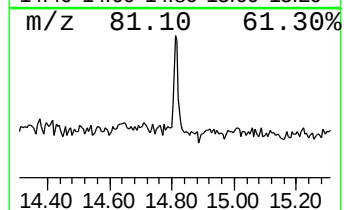
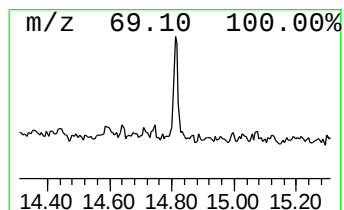
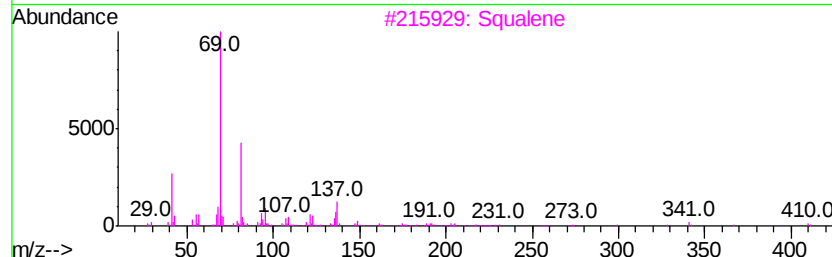
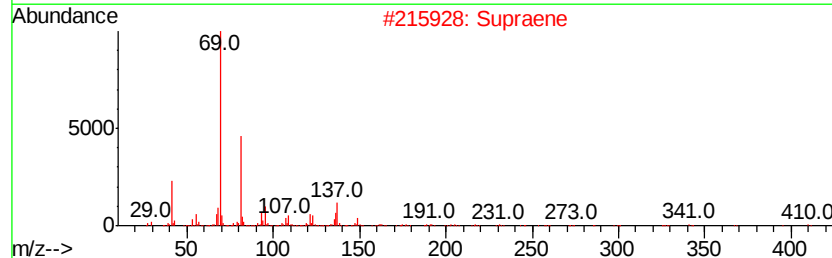
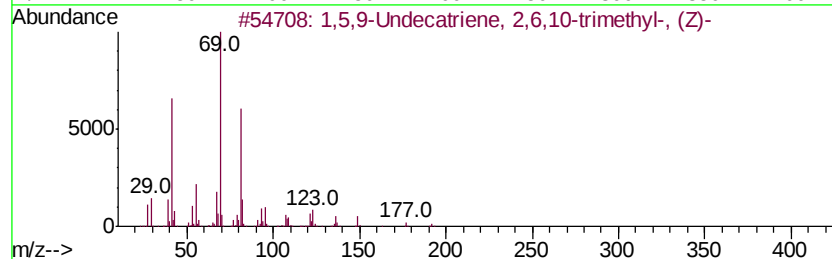
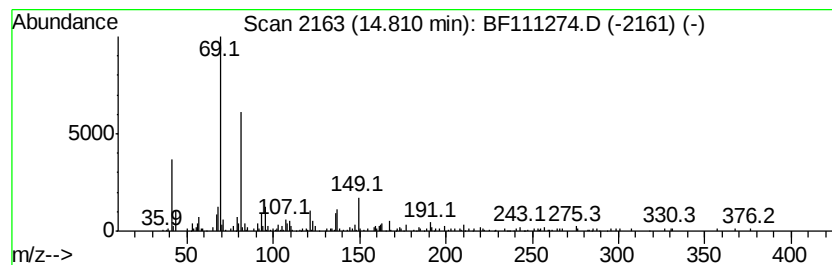
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1,5,9-Undecatriene, 2,6,10-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	2.39 ng	160869	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	81
2		Supraene	410	C30H50	007683-64-9	80
3		Squalene	410	C30H50	000111-02-4	80
4		2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	50
5		1,5-Heptadiene, 3,3,5-trimethyl-	138	C10H18	074630-29-8	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121118\
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.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...	5.02	5.8	ng	654641	1	6.80	2252960	20.0
2-Furanmethanol	5.17	12.2	ng	1373530	1	6.80	2252960	20.0
unknown6.57	6.57	90.6	ng	10210800	1	6.80	2252960	20.0
Mesitylene	6.63	2.5	ng	287391	1	6.80	2252960	20.0
n-Hexadecanoic acid	11.85	9.2	ng	1194520	4	11.32	2603710	20.0
Octadecanoic acid	12.63	3.3	ng	423364	4	11.32	2603710	20.0
unknown13.36	13.36	2.1	ng	183067	5	13.95	1729630	20.0
Pentafluoropropio...	13.81	4.7	ng	403714	5	13.95	1729630	20.0
1,5,9-Undecatrien...	14.81	2.4	ng	160869	6	15.39	1343400	20.0