

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061818\
 Data File : BF106542.D
 Acq On : 18 Jun 2018 16:54
 Operator : JU/SJ
 Sample : J3505-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-56-COMP

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-BF061118.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	5.201	483	487	497	rVB	191244	216639	1.13%	0.386%
2	5.613	553	557	570	rVB	2206457	2149154	11.19%	3.827%
3	6.607	722	726	743	rVB	2296206	2160403	11.24%	3.847%
4	6.742	745	749	753	rVB	2341000	2161119	11.25%	3.848%
5	6.966	783	787	790	rBV	959256	735673	3.83%	1.310%
6	7.125	809	814	817	rVB	1873241	1713097	8.92%	3.050%
7	7.525	878	882	886	rBV	1414248	1464901	7.62%	2.608%
8	8.248	1001	1005	1008	rBV	1103772	909318	4.73%	1.619%
9	9.319	1183	1187	1191	rBV	2455008	2385125	12.41%	4.247%
10	9.713	1250	1254	1258	rBV	405757	320036	1.67%	0.570%
11	10.007	1300	1304	1307	rBV	1118118	936521	4.87%	1.667%
12	10.801	1435	1439	1442	rBV	1302678	1222580	6.36%	2.177%
13	11.001	1470	1473	1476	rVB	512748	381090	1.98%	0.679%
14	11.495	1554	1557	1560	rBV	860549	799365	4.16%	1.423%
15	11.795	1606	1608	1613	rVB	634030	556541	2.90%	0.991%
16	11.889	1618	1624	1627	rBV	4472224	6757534	35.17%	12.032%
17	12.277	1687	1690	1697	rBV	239414	205157	1.07%	0.365%
18	12.618	1734	1748	1750	rBV4	4366348	19214101	100.00%	34.210%
19	12.654	1753	1754	1755	rVV	578259	315361	1.64%	0.561%
20	12.683	1755	1759	1762	rVB	3864929	3935525	20.48%	7.007%
21	12.965	1801	1807	1811	rVB6	135569	240239	1.25%	0.428%
22	13.089	1824	1828	1832	rBV	1987339	1814270	9.44%	3.230%
23	13.318	1861	1867	1873	rVB	1048289	1172219	6.10%	2.087%
24	13.395	1876	1880	1882	rBV	861266	710033	3.70%	1.264%
25	13.418	1882	1884	1889	rVV3	299396	320398	1.67%	0.570%
26	13.460	1889	1891	1896	rVV3	239589	255620	1.33%	0.455%
27	13.607	1913	1916	1919	rVB	241077	240751	1.25%	0.429%
28	13.830	1949	1954	1962	rVB2	326569	499395	2.60%	0.889%
29	14.065	1991	1994	1999	rVB	557873	534283	2.78%	0.951%
30	14.154	2005	2009	2012	rBV	904032	788166	4.10%	1.403%
31	14.712	2100	2104	2107	rBV	232379	243014	1.26%	0.433%
32	15.701	2267	2272	2278	rVB	634033	807051	4.20%	1.437%

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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-BF061118.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

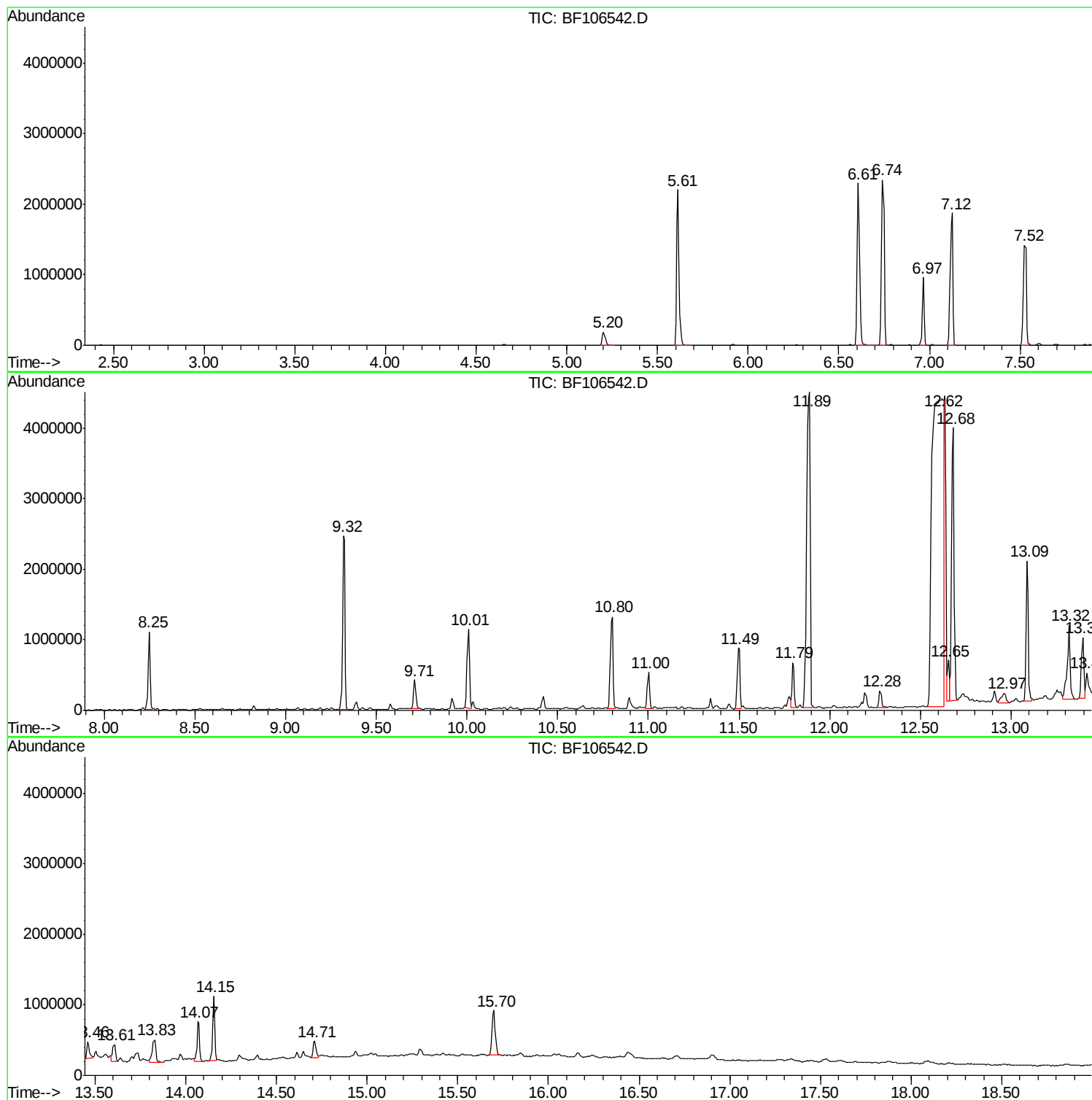
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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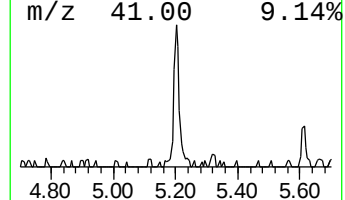
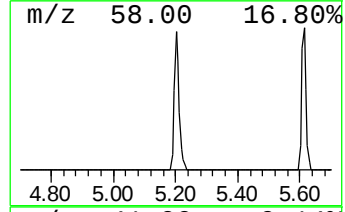
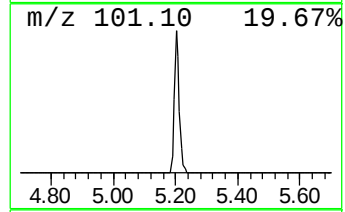
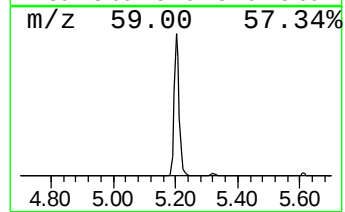
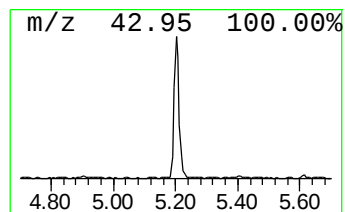
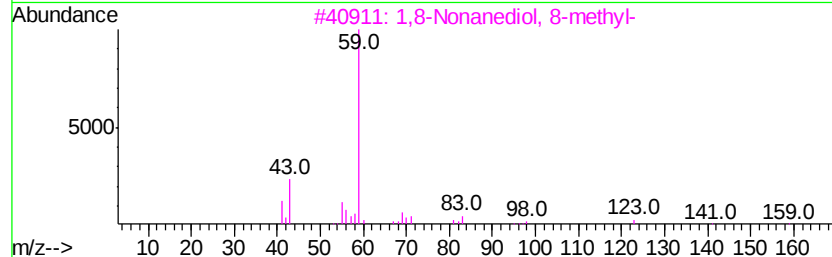
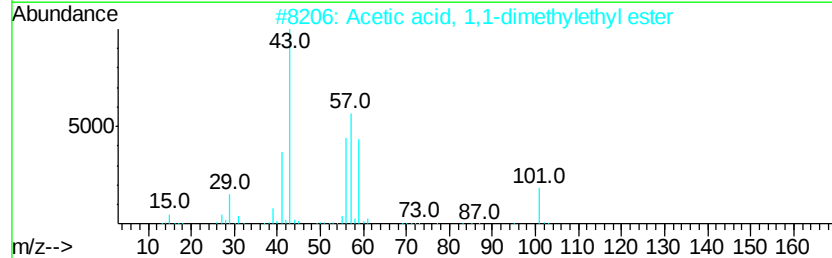
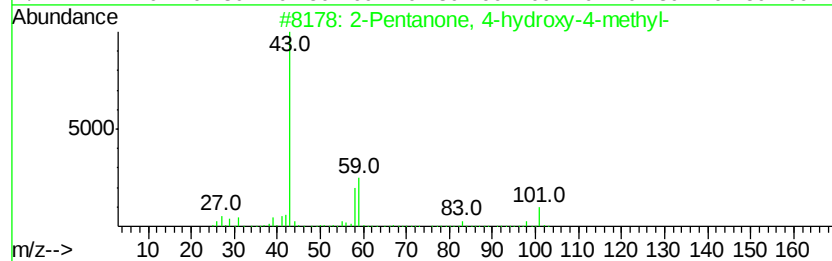
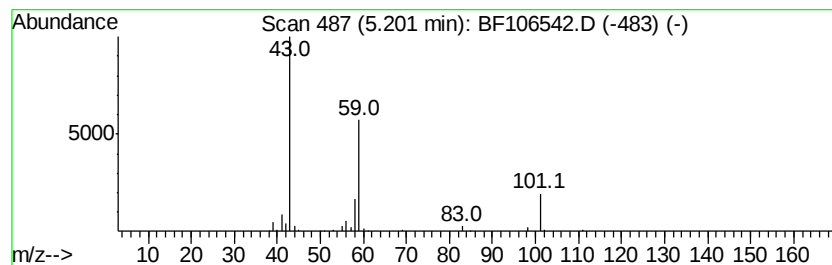
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	5.89 ng	216639	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17



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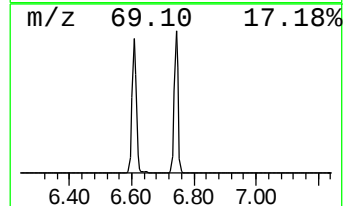
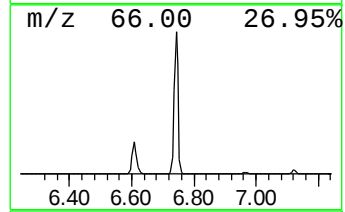
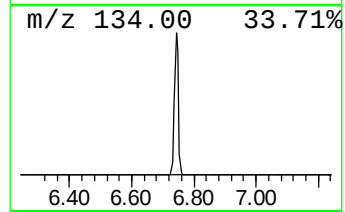
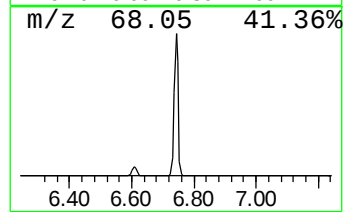
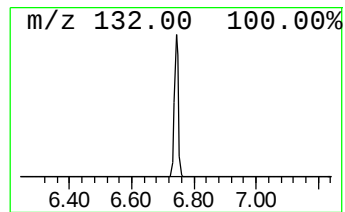
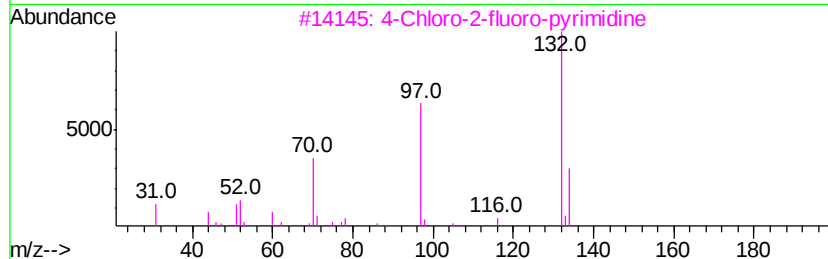
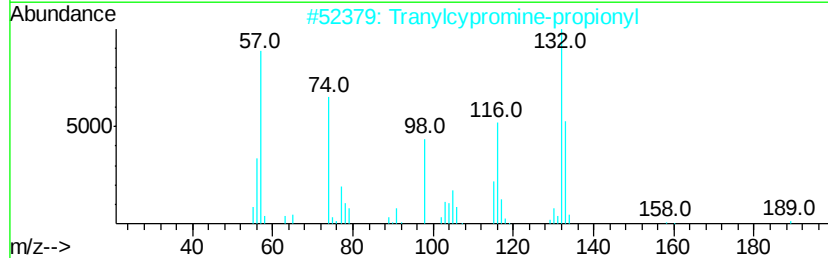
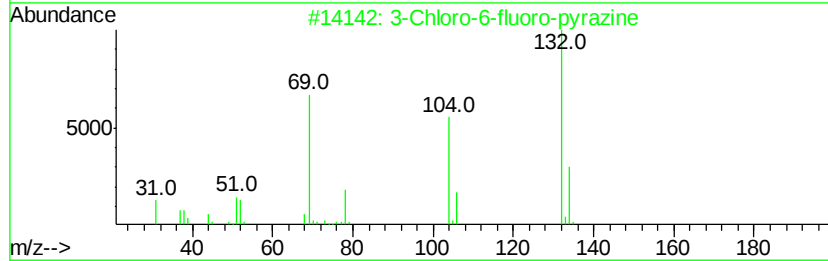
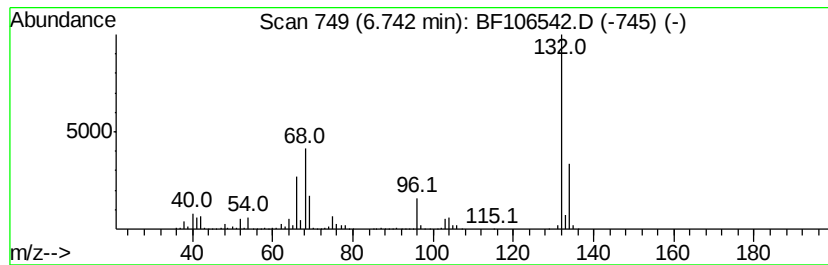
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.74 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	58.75 ng	2161120	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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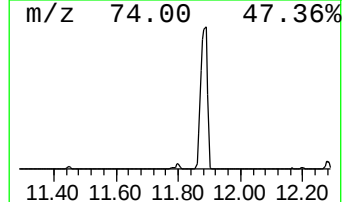
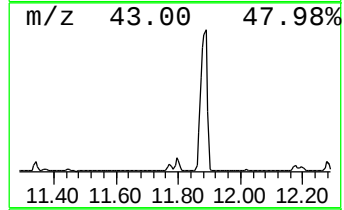
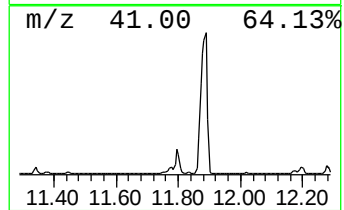
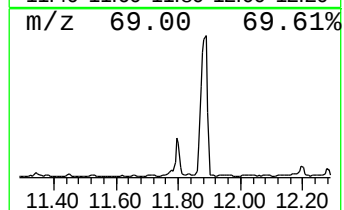
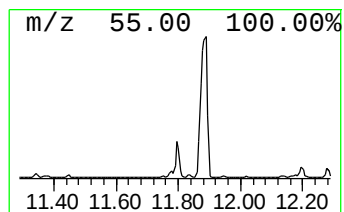
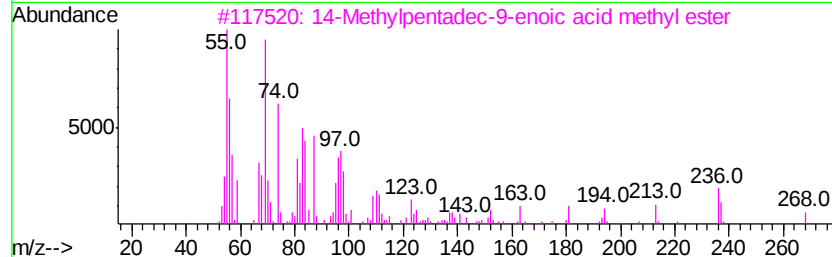
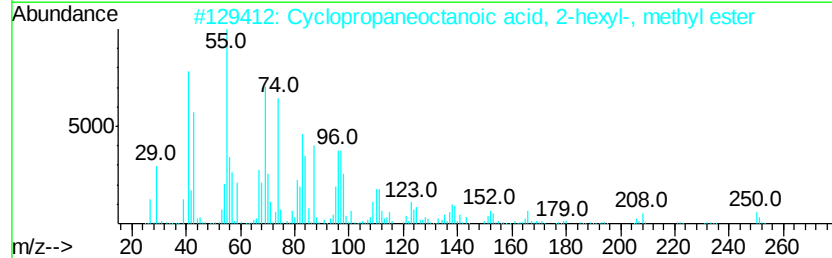
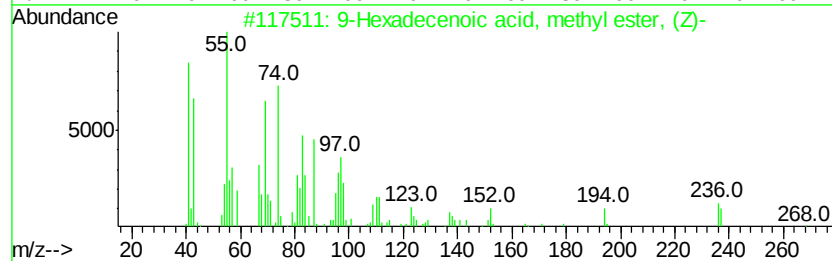
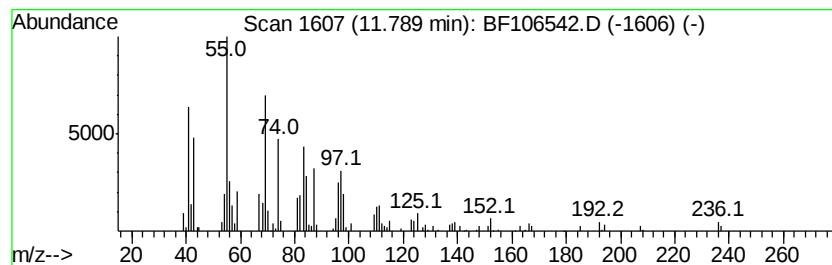
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Hexadecenoic acid, methyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	13.92 ng	556541	Phenanthrene-d10	11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	99
2		Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	91
3		14-Methylpentadec-9-enoic acid m...	268	C17H32O2	1000365-89-7	91
4		Methyl hexadec-9-enoate	268	C17H32O2	010030-74-7	90
5		9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	90



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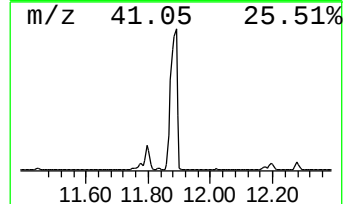
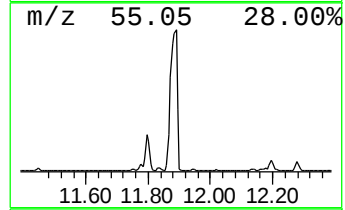
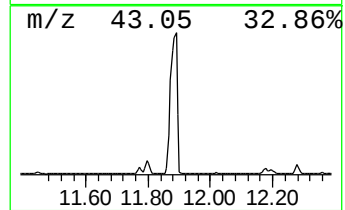
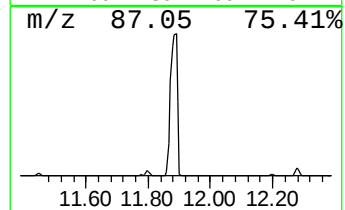
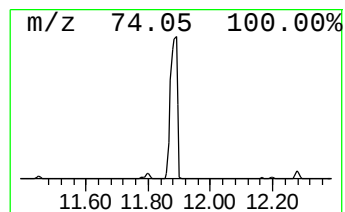
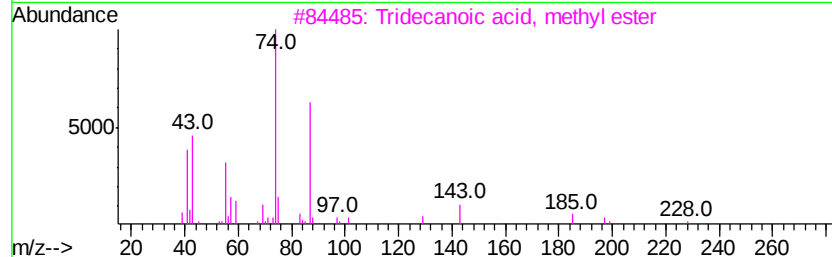
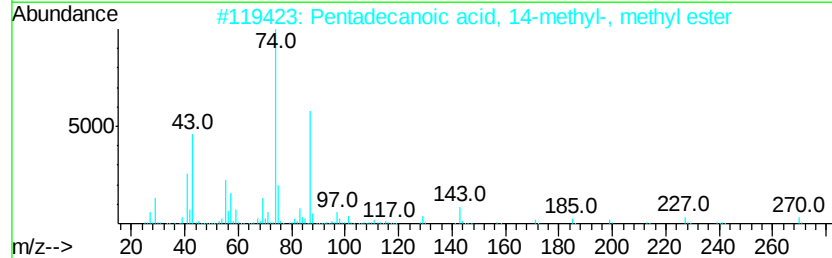
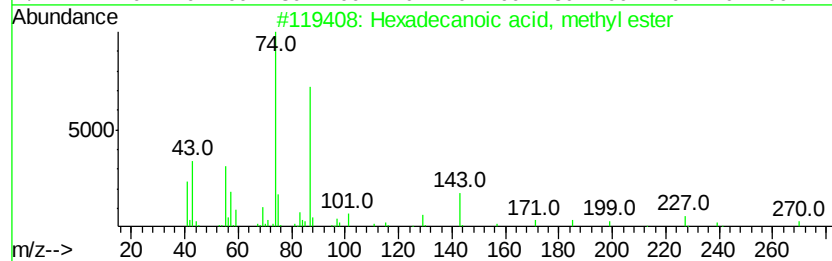
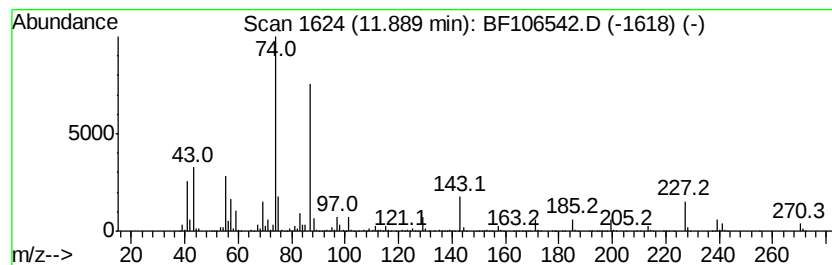
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Hexadecanoic acid, methyl e... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	169.07 ng	6757530	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4		Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	87
5		Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	87



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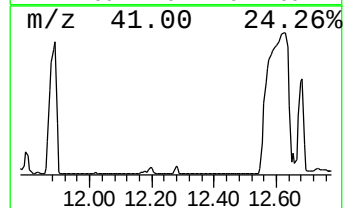
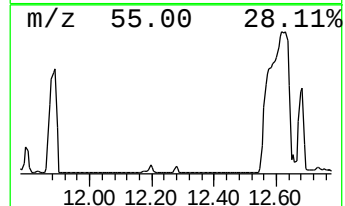
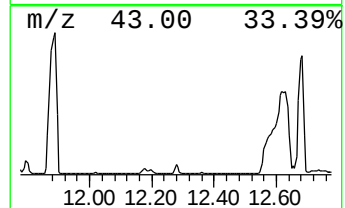
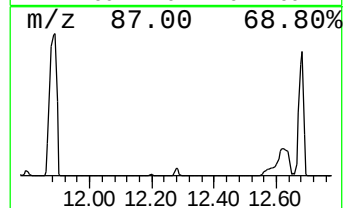
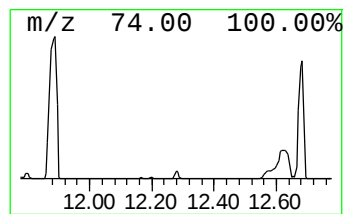
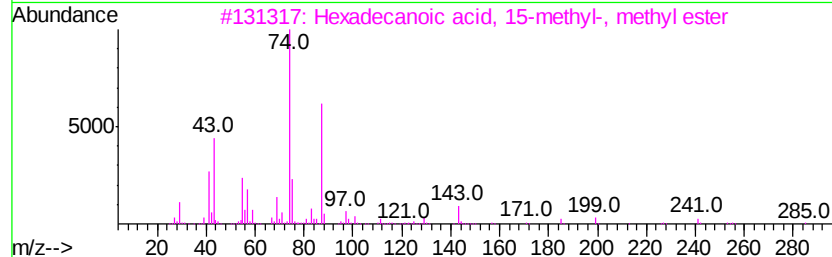
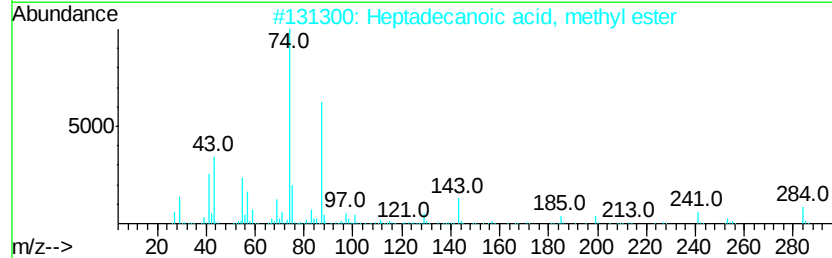
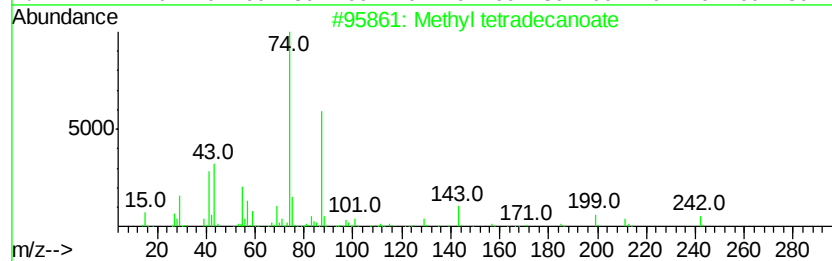
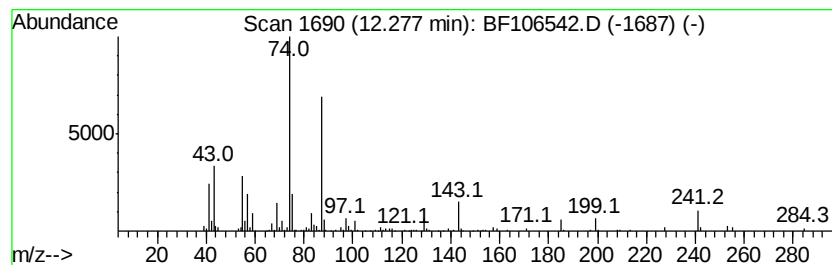
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TIC Integration Parameters: LSCINT.P

Peak Number 7 Methyl tetradecanoate Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.28	5.13 ng	205157	Phenanthrene-d10	11.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
2			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
3			Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	90
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	86



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Data File : BF106542.D
Acq On : 18 Jun 2018 16:54
Operator : JU/SJ
Sample : J3505-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-56-COMP

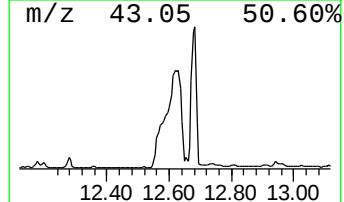
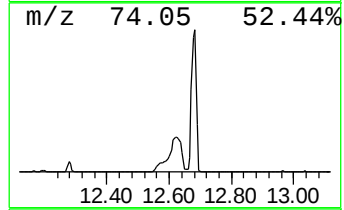
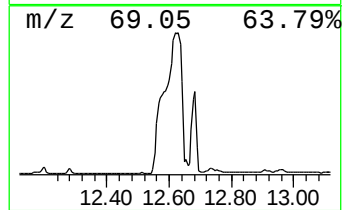
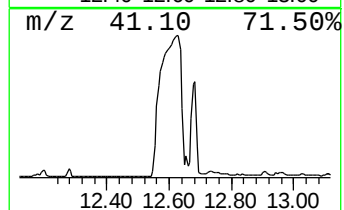
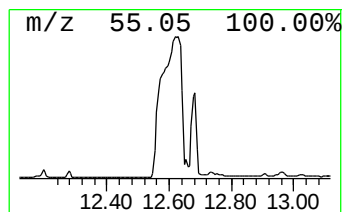
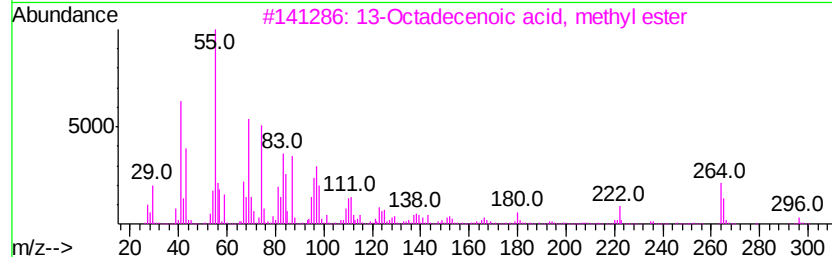
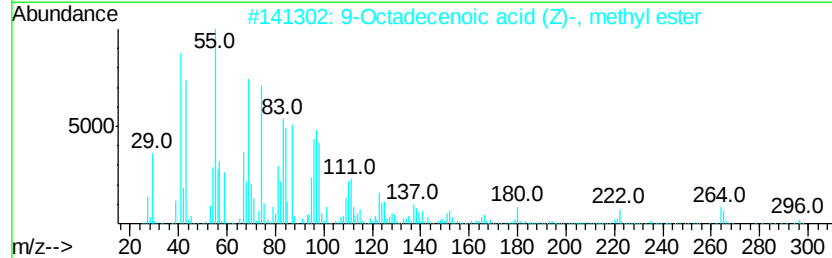
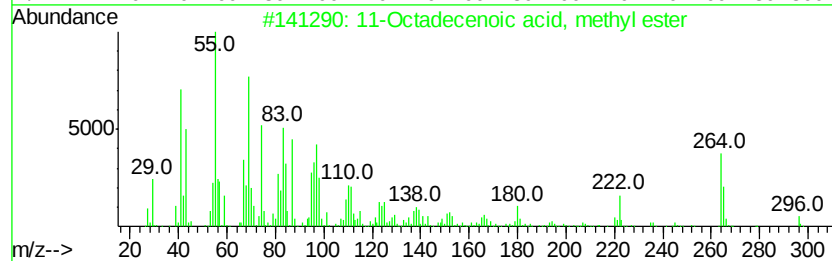
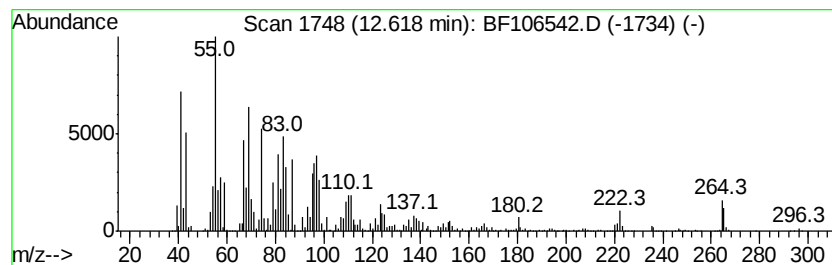
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 11-Octadecenoic acid, methyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.62	480.73 ng	19214100	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
2		9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
3		13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
4		12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
5		14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061818\
Data File : BF106542.D
Acq On : 18 Jun 2018 16:54
Operator : JU/SJ
Sample : J3505-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-56-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9,12,15-Octadecatrienoic ac... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	7.89 ng	315361	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9,12,15-Octadecatrienoic acid, m...	292	C19H32O2	000301-00-8	93
2		9,12,15-Octadecatrienoic acid, (...	278	C18H30O2	000463-40-1	87
3		3-Undecen-1-yne, (Z)-	150	C11H18	074744-32-4	64
4		3-Dodecen-1-yne, (Z)-	164	C12H20	025091-24-1	64
5		9-Octadecen-12-ynoic acid, methy...	292	C19H32O2	056847-05-3	64

