

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062218\
 Data File : BF106699.D
 Acq On : 22 Jun 2018 10:51
 Operator : JU/SJ
 Sample : J3603-11
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 26KV-CSM

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-BF061918.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	5.207	484	488	497	rBV	114658	148224	7.34%	0.924%
2	5.607	552	556	560	rBV	1527410	1469903	72.80%	9.165%
3	6.607	721	726	729	rBV	1434096	1520461	75.30%	9.481%
4	6.742	744	749	752	rBV	1464351	1532650	75.91%	9.557%
5	6.778	752	755	761	rVB	46139	36871	1.83%	0.230%
6	6.960	782	786	789	rBV	464487	362791	17.97%	2.262%
7	7.119	808	813	816	rBV	1349477	1246388	61.73%	7.772%
8	7.525	876	882	885	rBV	1038614	1050456	52.03%	6.550%
9	8.242	1000	1004	1008	rBV	554627	459243	22.74%	2.864%
10	9.319	1182	1187	1190	rBV	1877491	1839517	91.11%	11.470%
11	9.707	1249	1253	1261	rBV	215961	169323	8.39%	1.056%
12	10.001	1299	1303	1307	rBV	644276	539982	26.74%	3.367%
13	10.413	1371	1373	1376	rVB	36747	25506	1.26%	0.159%
14	10.801	1434	1439	1442	rBV	1200978	1309028	64.83%	8.162%
15	10.883	1450	1453	1458	rBV	42293	39419	1.95%	0.246%
16	11.336	1523	1530	1532	rBV	21461	20216	1.00%	0.126%
17	11.495	1553	1557	1560	rBV	679905	588836	29.16%	3.672%
18	12.954	1795	1805	1811	rBV3	20985	28057	1.39%	0.175%
19	13.083	1822	1827	1830	rBV	2036105	2019104	100.00%	12.590%
20	13.601	1911	1915	1918	rBV	468472	424281	21.01%	2.646%
21	13.954	1972	1975	1981	rBV2	136752	152543	7.55%	0.951%
22	14.148	2003	2008	2011	rBV	516457	501090	24.82%	3.124%
23	14.601	2081	2085	2093	rBV8	23825	38802	1.92%	0.242%
24	15.607	2253	2256	2263	rBV7	13806	22675	1.12%	0.141%
25	15.683	2264	2269	2280	rVB	356879	471359	23.34%	2.939%
26	16.712	2441	2444	2450	rVB	12801	20883	1.03%	0.130%

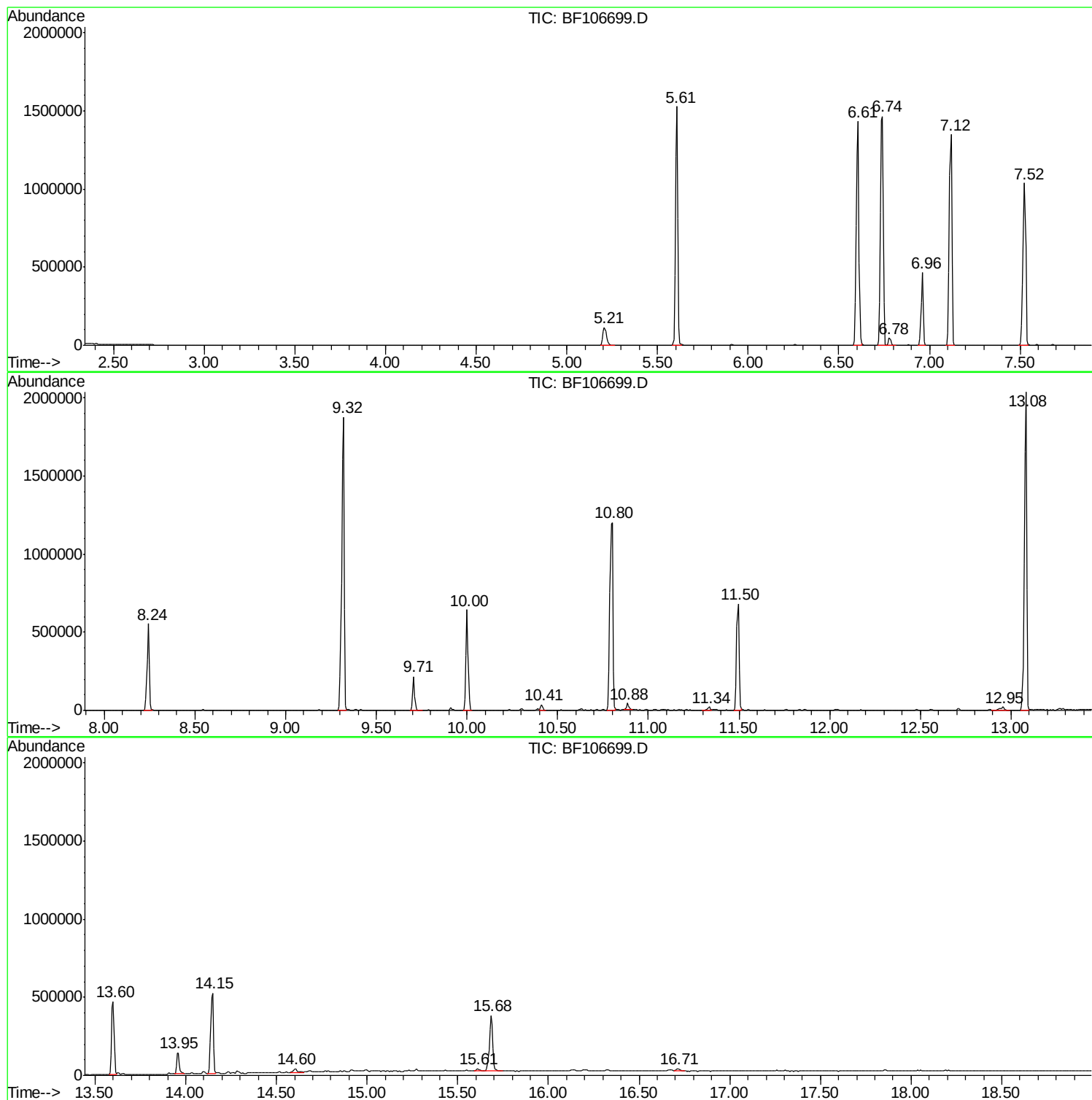
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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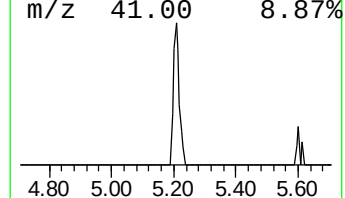
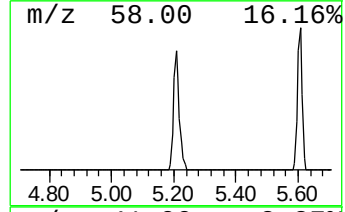
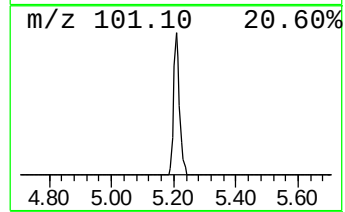
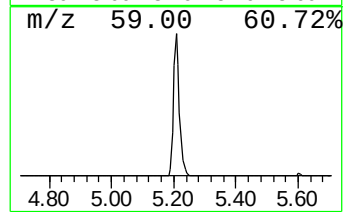
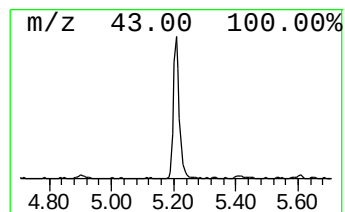
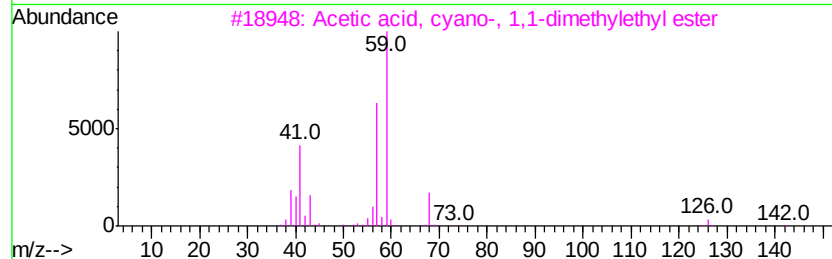
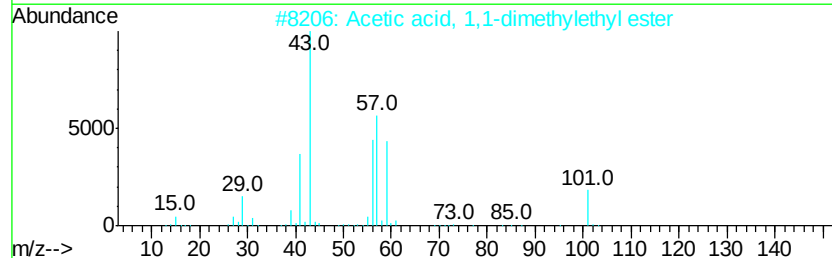
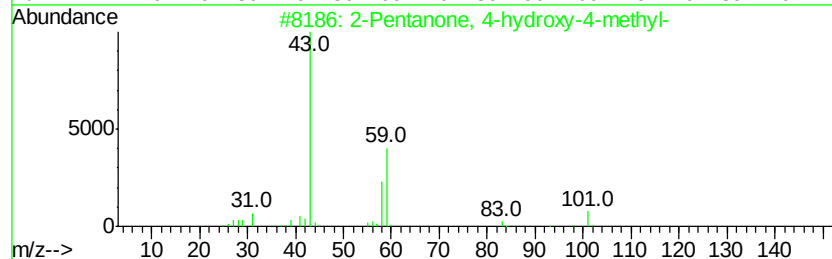
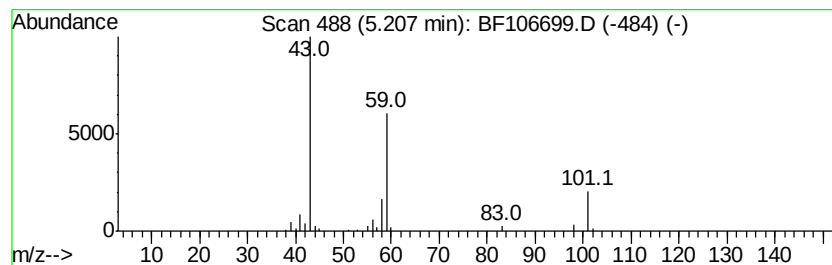
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	8.17 ng	148224	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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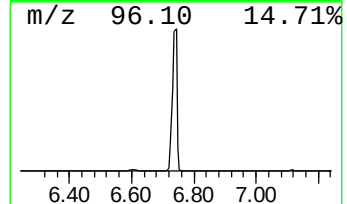
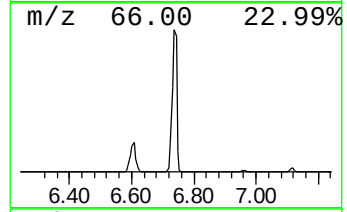
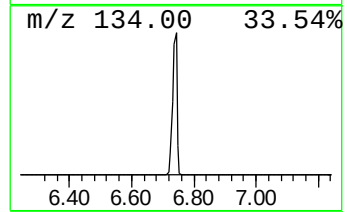
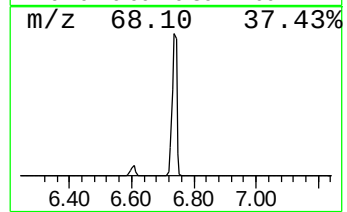
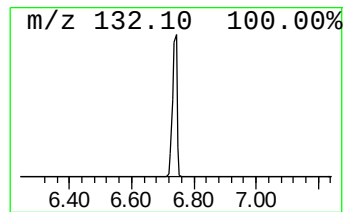
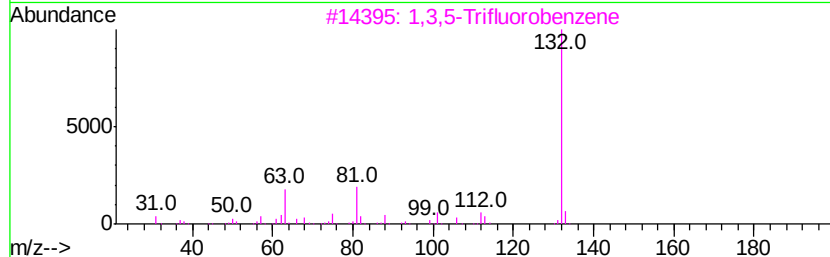
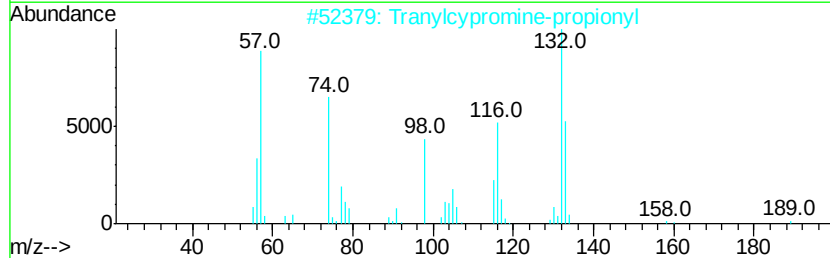
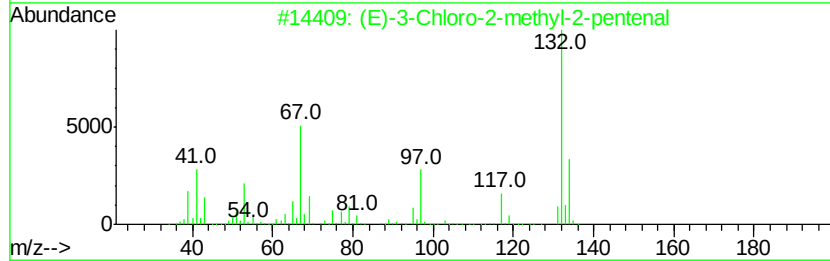
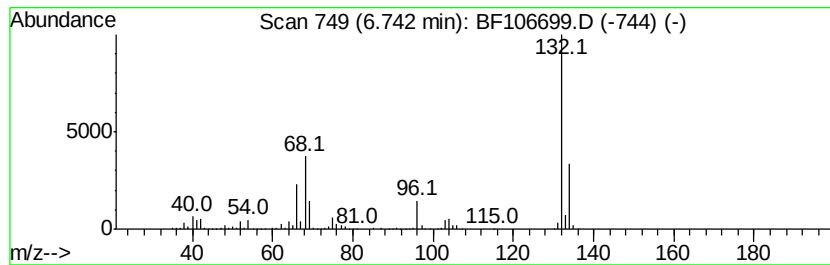
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	84.49 ng	1532650	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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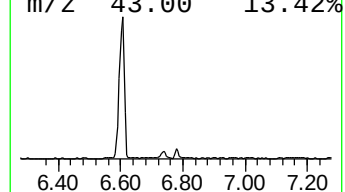
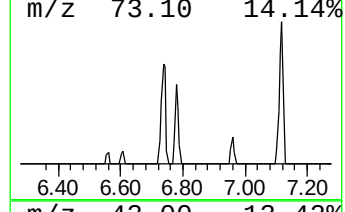
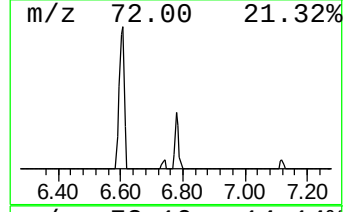
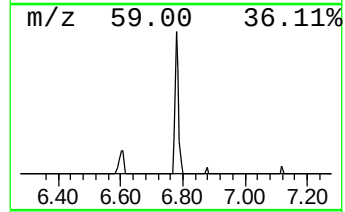
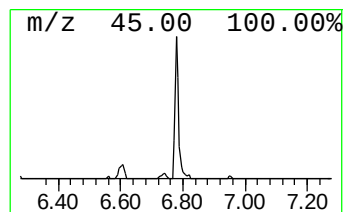
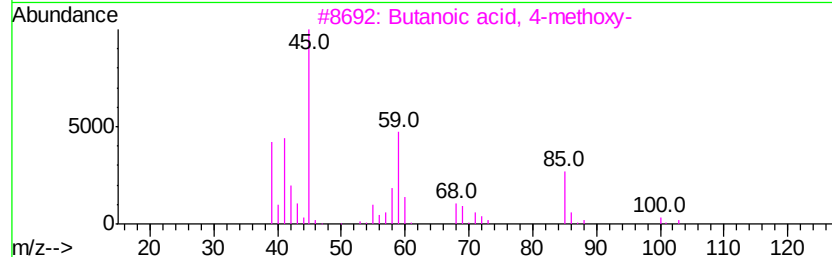
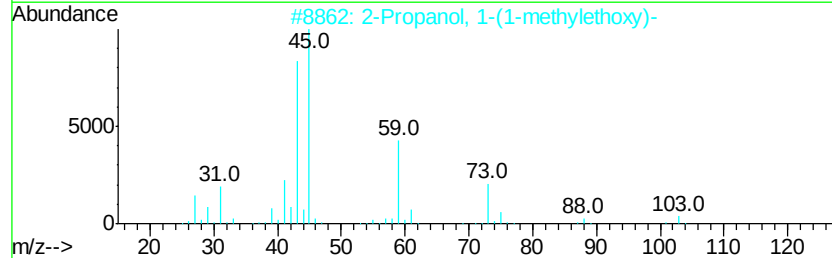
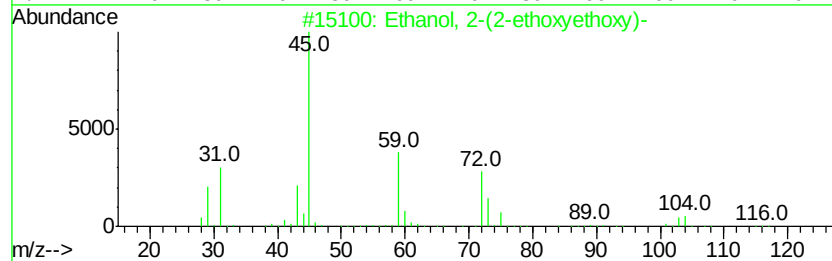
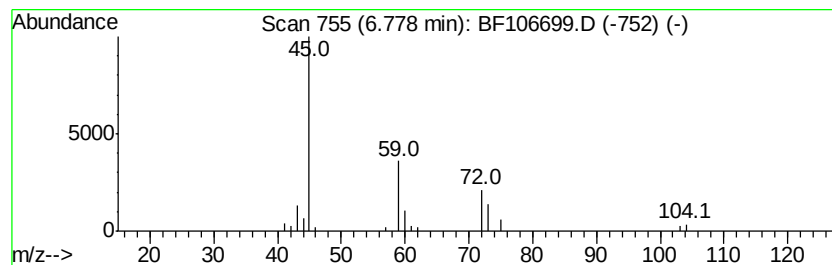
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Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	2.03 ng	36871	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2		2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
3		Butanoic acid, 4-methoxy-	118	C5H10O3	029006-02-8	38
4		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	23
5		2-Hydroxyethyl vinyl sulfide	104	C4H8OS	003090-56-0	9



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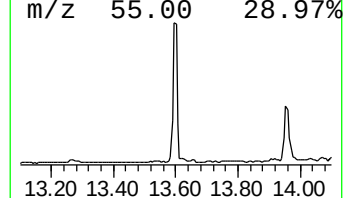
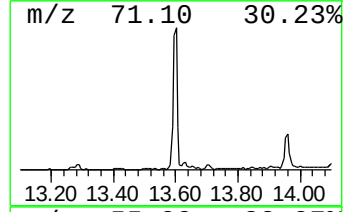
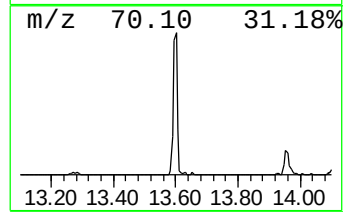
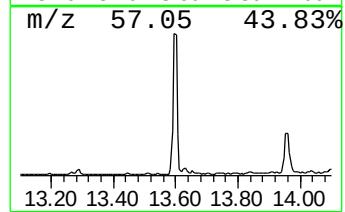
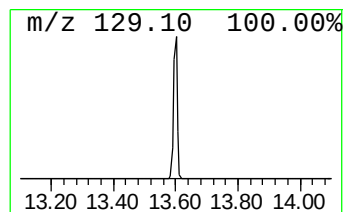
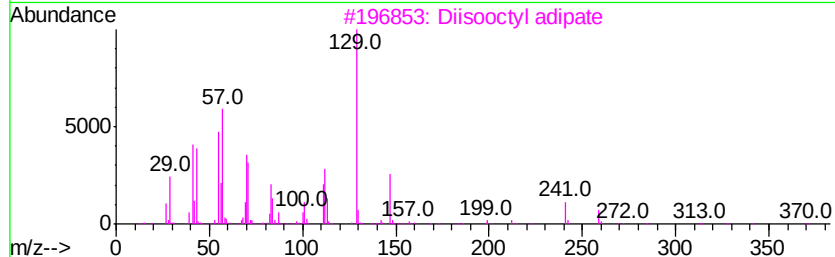
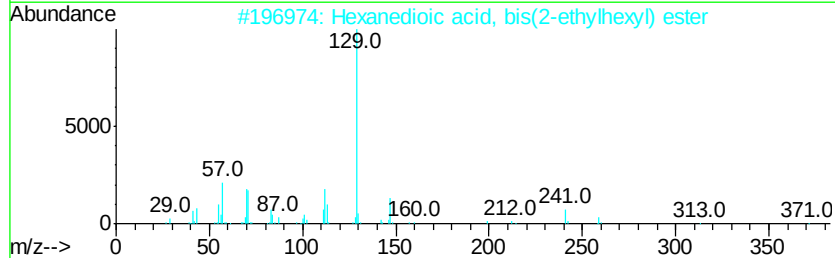
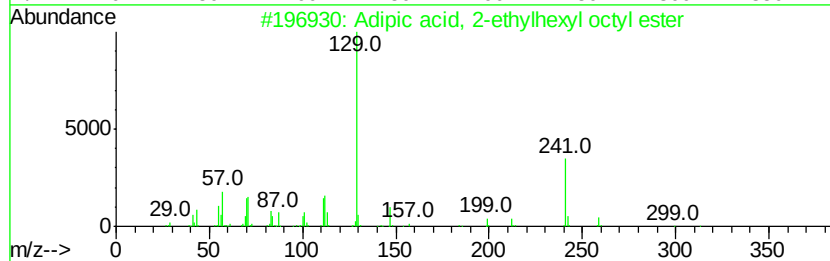
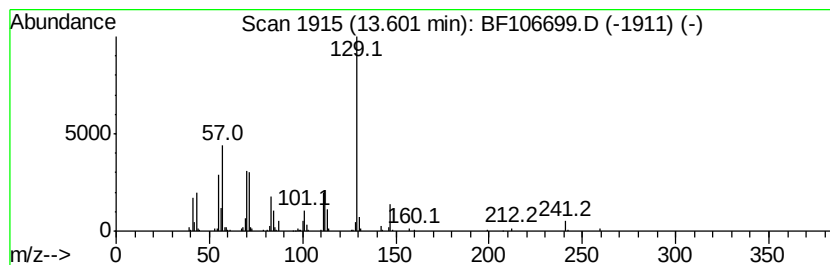
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Peak Number 5 Adipic acid, 2-ethylhexyl o... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.60	16.93 ng	424281	Chrysene-d12	14.15	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	91
2	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	87
3	Diisooctyl adipate	370	C22H42O4	001330-86-5	78
4	Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1000324-48-0	72
5	Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	68



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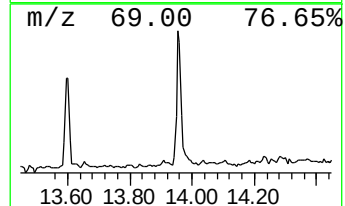
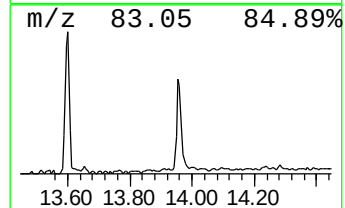
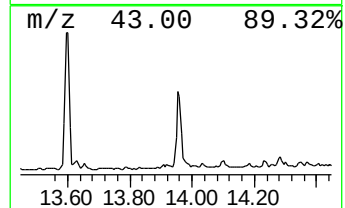
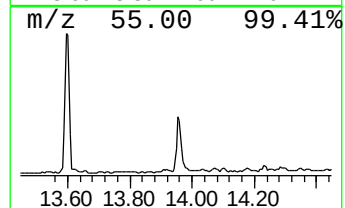
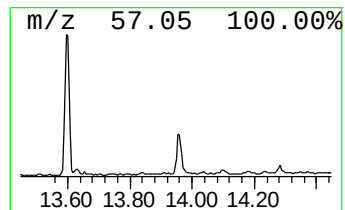
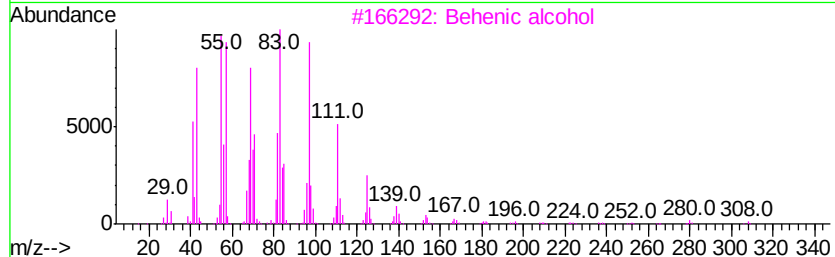
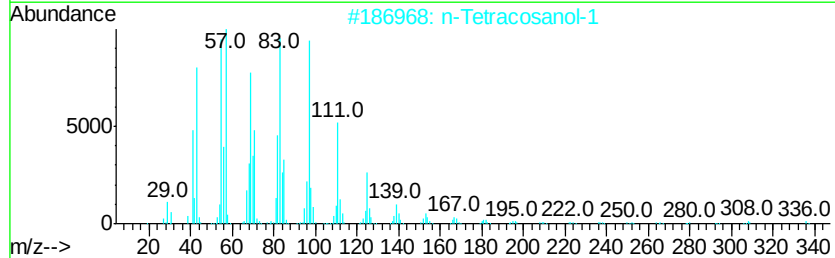
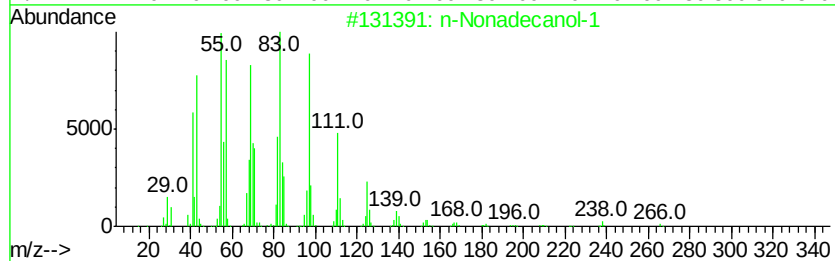
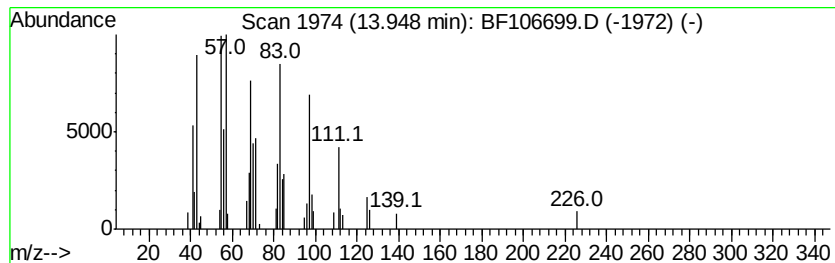
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.95	6.09 ng	152543	Chrysene-d12	14.15	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	94
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.21	8.2	ng	148224	1	6.96	362791	20.0
unknown6.74	6.74	84.5	ng	1532650	1	6.96	362791	20.0
Ethanol, 2-(2-eth...	6.78	2.0	ng	36871	1	6.96	362791	20.0
Adipic acid, 2-et...	13.60	16.9	ng	424281	5	14.15	501090	20.0
n-Nonadecanol-1	13.95	6.1	ng	152543	5	14.15	501090	20.0