

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041318\
 Data File : BF104498.D
 Acq On : 14 Apr 2018 00:02
 Operator : JU/SJ
 Sample : PB108229BL
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB108229BL

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:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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	5.016	494	498	505	rVB	75950	90621	4.29%	0.498%
2	5.428	564	568	571	rBV	1925178	1814419	85.83%	9.966%
3	5.751	619	623	632	rVB	54732	52616	2.49%	0.289%
4	6.445	736	741	744	rBV	1791801	1785309	84.46%	9.806%
5	6.581	759	764	767	rBV	2232391	1882698	89.06%	10.341%
6	6.810	799	803	806	rBV	998013	780376	36.92%	4.287%
7	6.963	825	829	833	rBV	1751899	1532972	72.52%	8.420%
8	7.375	894	899	902	rBV	1222857	1138935	53.88%	6.256%
9	8.092	1017	1021	1024	rBV	1264773	979118	46.32%	5.378%
10	9.169	1199	1204	1207	rBV	2535107	2113904	100.00%	11.611%
11	9.563	1267	1271	1274	rBV	116987	98684	4.67%	0.542%
12	9.775	1304	1307	1311	rBV	63811	47319	2.24%	0.260%
13	9.851	1316	1320	1328	rVB	1140102	986740	46.68%	5.420%
14	10.275	1389	1392	1395	rVB	83675	60254	2.85%	0.331%
15	10.492	1423	1429	1432	rBV	18273	24667	1.17%	0.135%
16	10.639	1450	1454	1463	rVB	1061693	897139	42.44%	4.928%
17	10.751	1470	1473	1478	rBV	60447	62393	2.95%	0.343%
18	11.339	1569	1573	1576	rBV	948373	797363	37.72%	4.380%
19	12.927	1839	1843	1846	rBV	1661478	1472058	69.64%	8.086%
20	13.821	1991	1995	1998	rBV	168338	178952	8.47%	0.983%
21	13.851	1998	2000	2004	rVB	138431	108515	5.13%	0.596%
22	13.980	2018	2022	2026	rBV	747078	674831	31.92%	3.707%
23	14.833	2164	2167	2170	rVB	40581	40342	1.91%	0.222%
24	15.451	2266	2272	2281	rBV	408461	530192	25.08%	2.912%
25	15.904	2345	2349	2353	rBV3	17740	25016	1.18%	0.137%
26	15.962	2355	2359	2365	rVB7	16897	29978	1.42%	0.165%

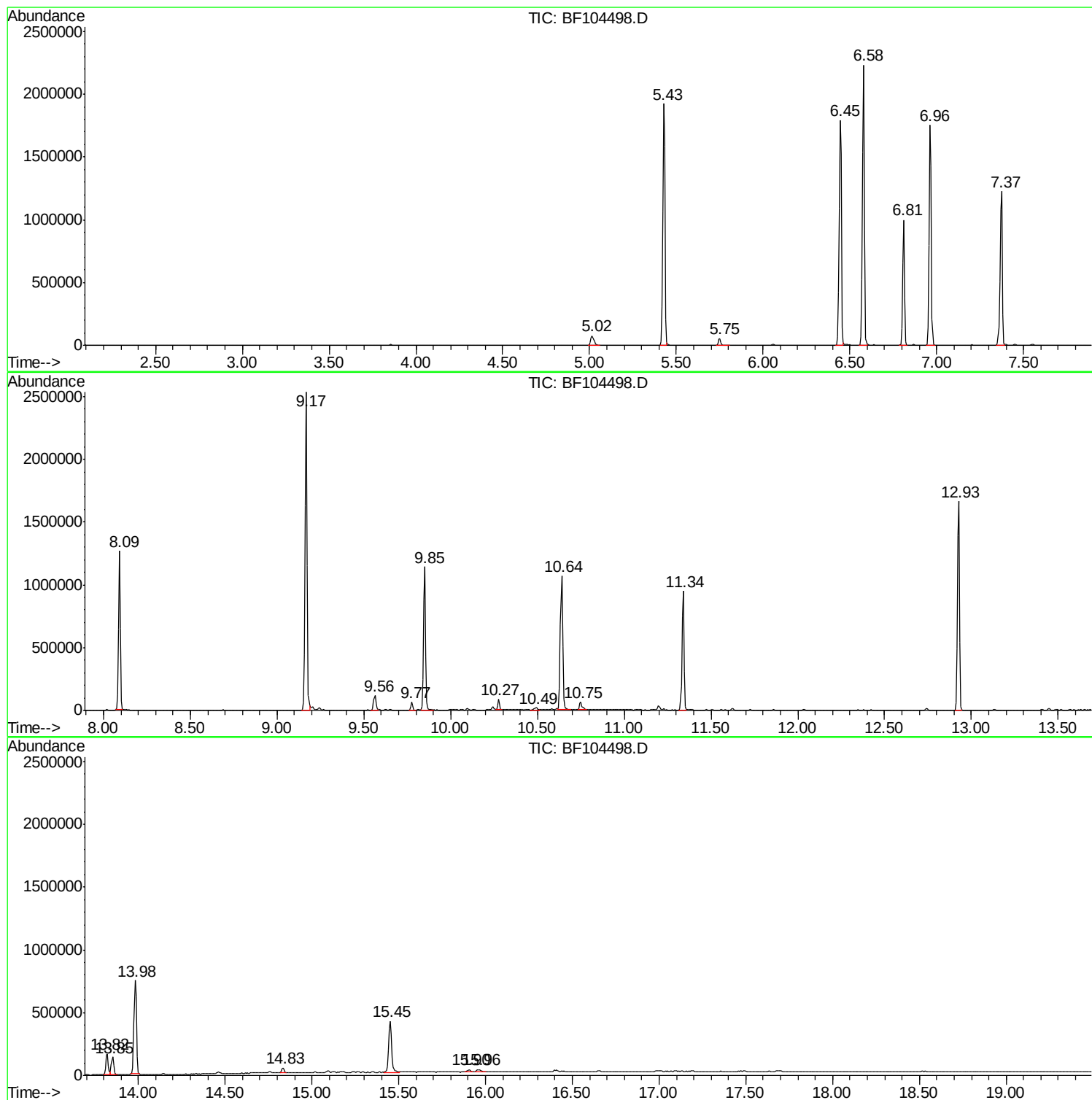
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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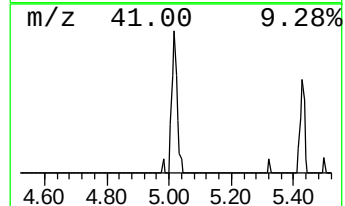
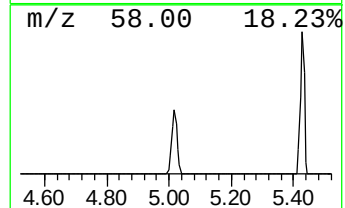
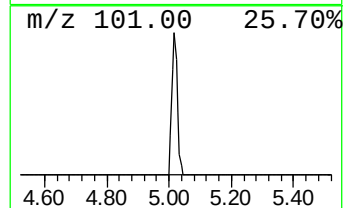
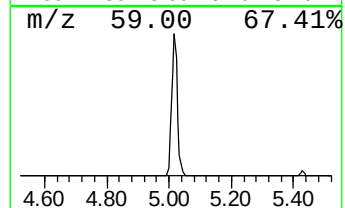
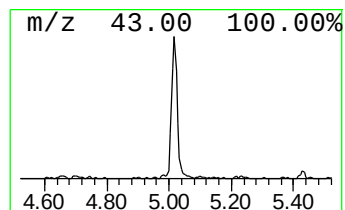
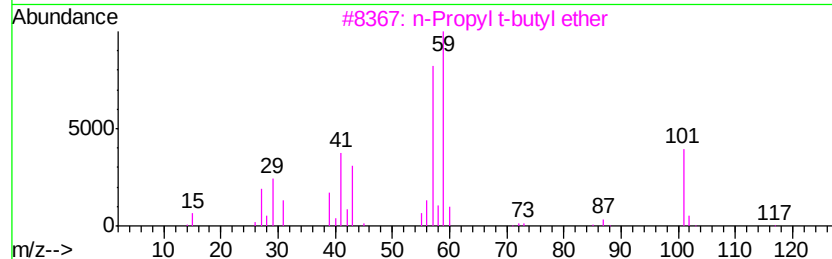
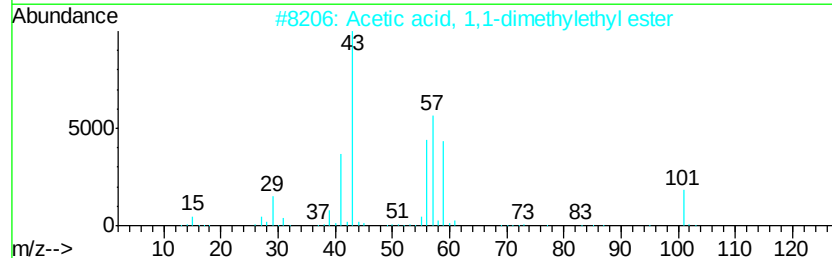
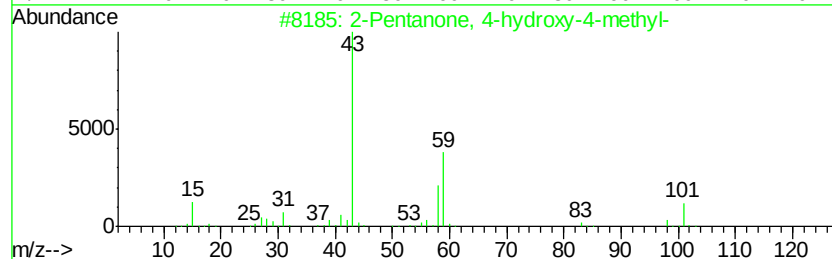
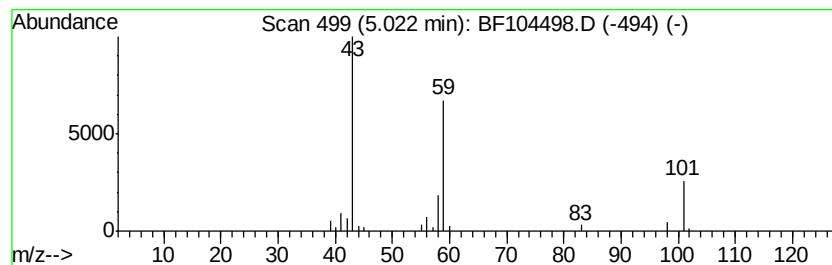
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	2.32 ng	90621	1,4-Dichlorobenzene-d4	6.81

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	38	
3	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33	
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17	
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	



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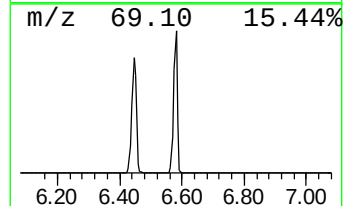
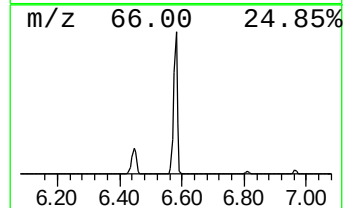
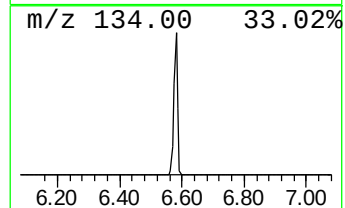
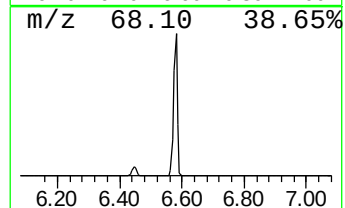
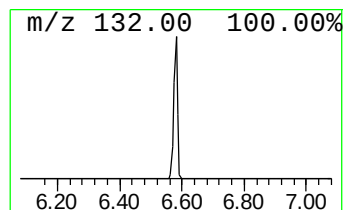
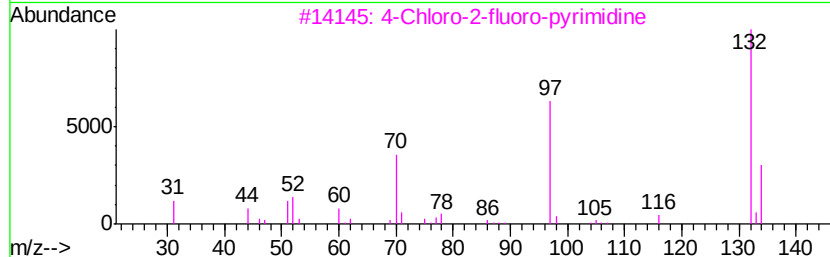
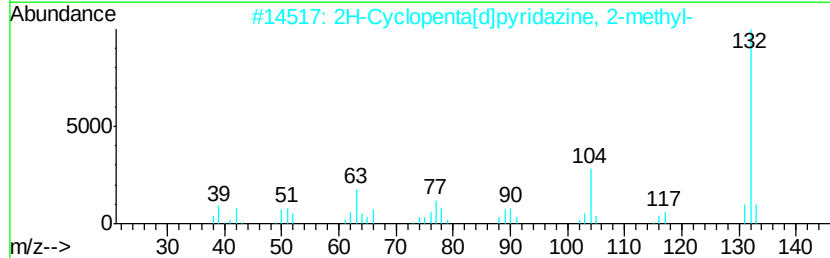
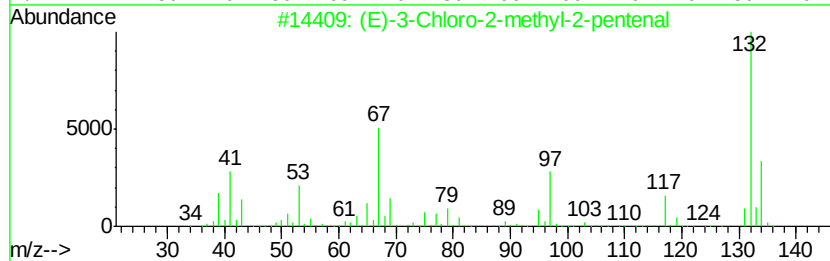
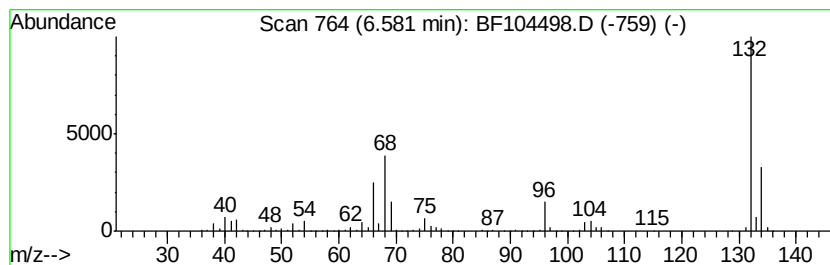
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Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	48.25 ng	1882700	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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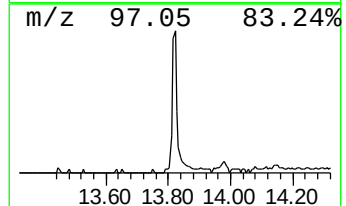
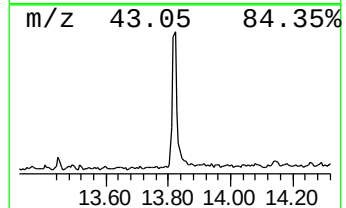
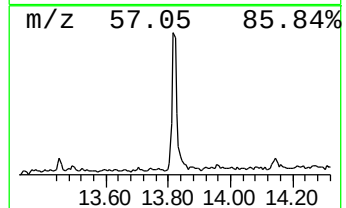
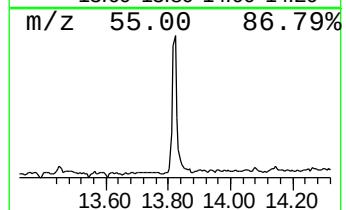
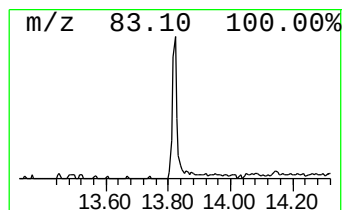
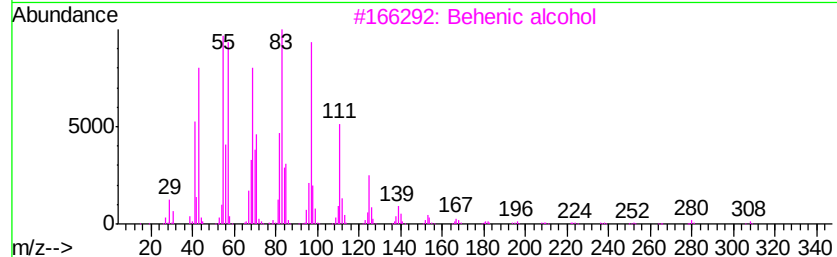
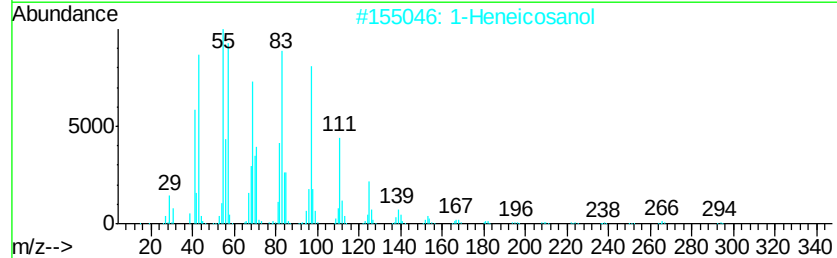
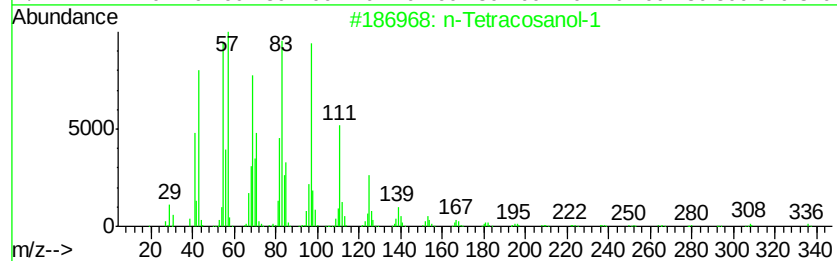
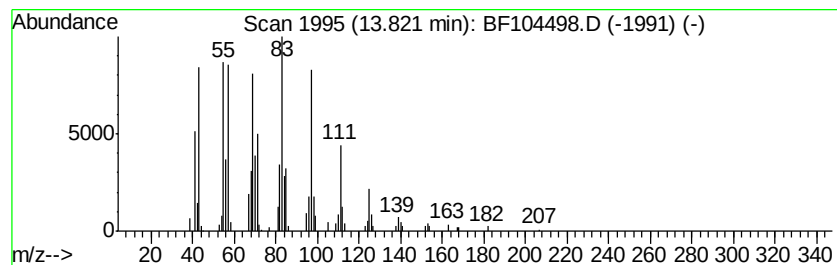
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Peak Number 4 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	5.30 ng	178952	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		Behenic alcohol	326	C22H46O	000661-19-8	95
4		1-Nonadecene	266	C19H38	018435-45-5	94
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93



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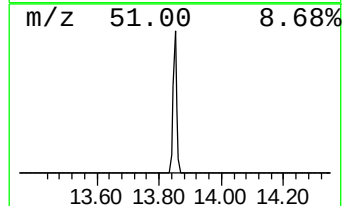
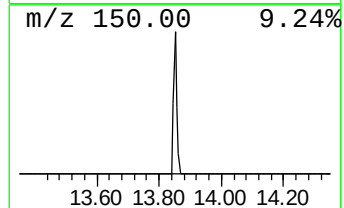
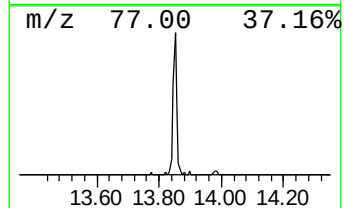
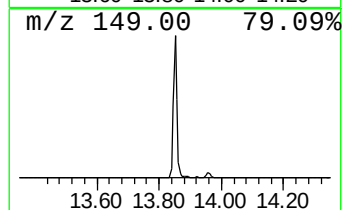
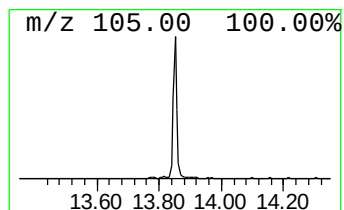
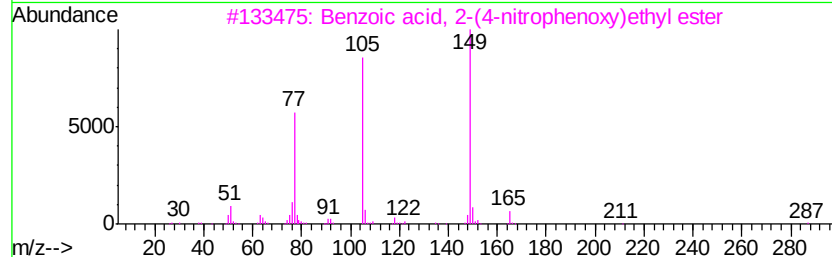
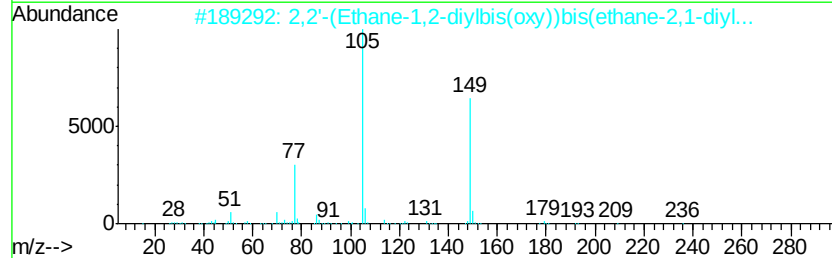
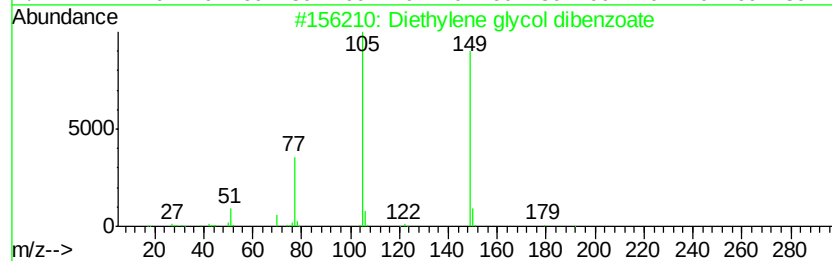
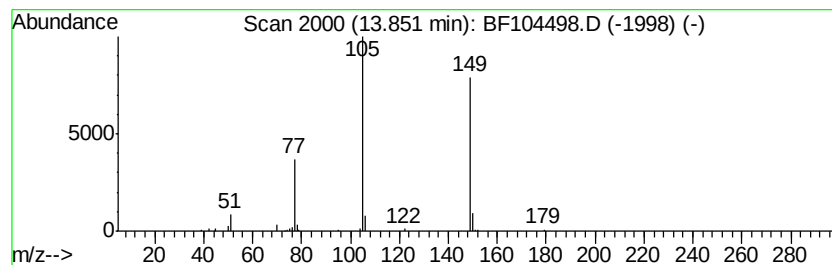
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Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.85	3.22 ng	108515	Chrysene-d12	13.98	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2	2,2'-(Ethane-1,2-diylbis(oxv))bi...	358	C20H22O6	1000366-99-4	83
3	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	78
4	2,5,8,11-Tetraoxatridecan-13-yl ...	312	C16H24O6	1000366-96-7	78
5	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	78



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	2.3	ng	90621	1	6.81	780376	20.0
unknown6.58	6.58	48.3	ng	1882700	1	6.81	780376	20.0
n-Tetracosanol-1	13.82	5.3	ng	178952	5	13.98	674831	20.0
Diethylene glycol...	13.85	3.2	ng	108515	5	13.98	674831	20.0