

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030122\
 Data File : BF127119.D
 Acq On : 01 Mar 2022 16:38
 Operator : CG\JU
 Sample : N1688-09
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-26

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-BF021622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127119.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.222	154	159	164	rBV2	31509	53886	1.67%	0.306%
2	5.504	543	547	551	rBV	1473554	1331466	41.25%	7.560%
3	6.516	715	719	730	rVB	965665	942986	29.21%	5.354%
4	6.887	779	782	786	rBV	634483	545680	16.90%	3.098%
5	7.457	873	879	882	rVB	1929313	1759780	54.51%	9.992%
6	7.739	922	927	930	rVB2	75412	70002	2.17%	0.397%
7	8.069	980	983	989	rBV2	57582	73318	2.27%	0.416%
8	8.175	997	1001	1004	rBV	891193	731434	22.66%	4.153%
9	8.575	1066	1069	1078	rVB8	19602	44853	1.39%	0.255%
10	9.251	1178	1184	1187	rBV	3980958	3228097	100.00%	18.328%
11	9.828	1278	1282	1288	rBV	107958	104127	3.23%	0.591%
12	9.933	1294	1300	1303	rBV	978206	834786	25.86%	4.740%
13	10.727	1430	1435	1438	rBV	2619115	2478628	76.78%	14.073%
14	11.422	1549	1553	1557	rBV	1050661	839378	26.00%	4.766%
15	11.598	1577	1583	1587	rBV2	87045	115262	3.57%	0.654%
16	11.939	1637	1641	1645	rBV	117012	118608	3.67%	0.673%
17	11.974	1645	1647	1650	rVB	62152	53986	1.67%	0.307%
18	13.016	1819	1824	1827	rBV	3185890	3109195	96.32%	17.653%
19	13.927	1971	1979	1987	rBV2	137847	244887	7.59%	1.390%
20	14.068	1999	2003	2006	rBV	556399	486726	15.08%	2.763%
21	15.562	2252	2257	2263	rVB	374245	445650	13.81%	2.530%

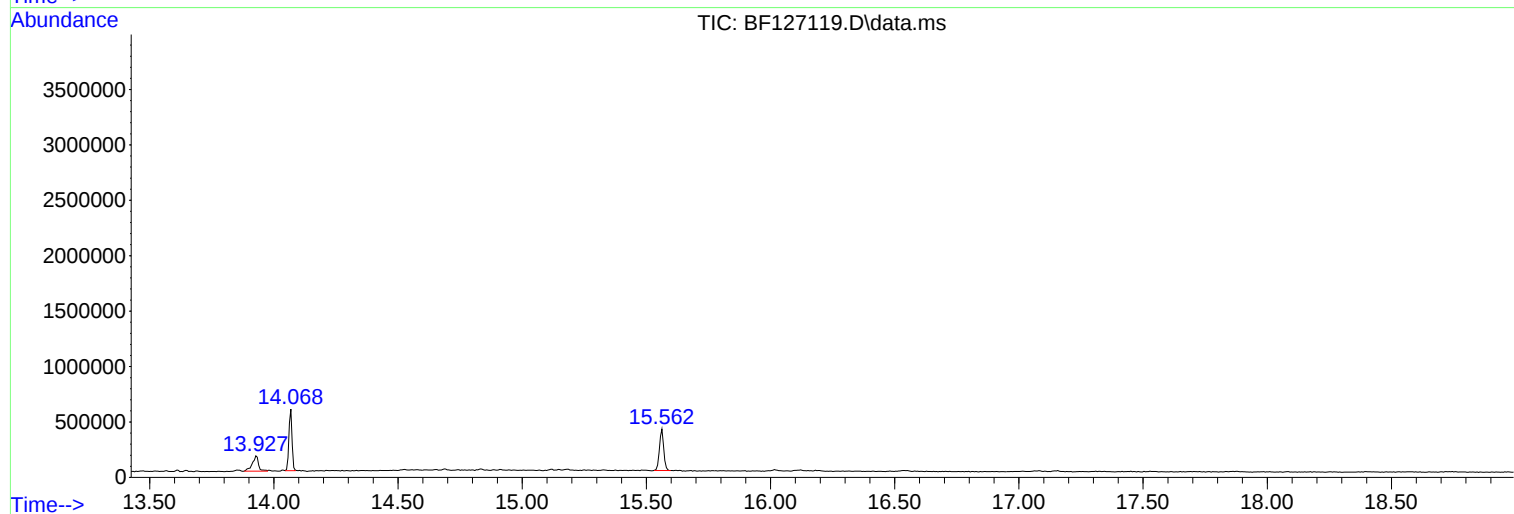
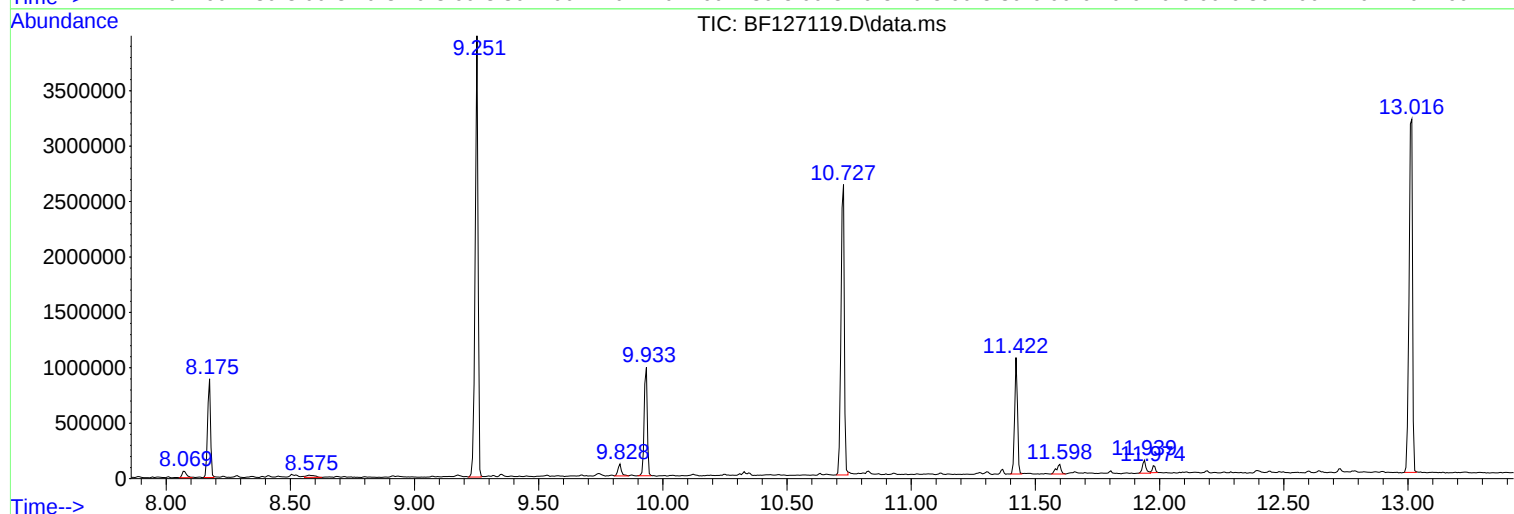
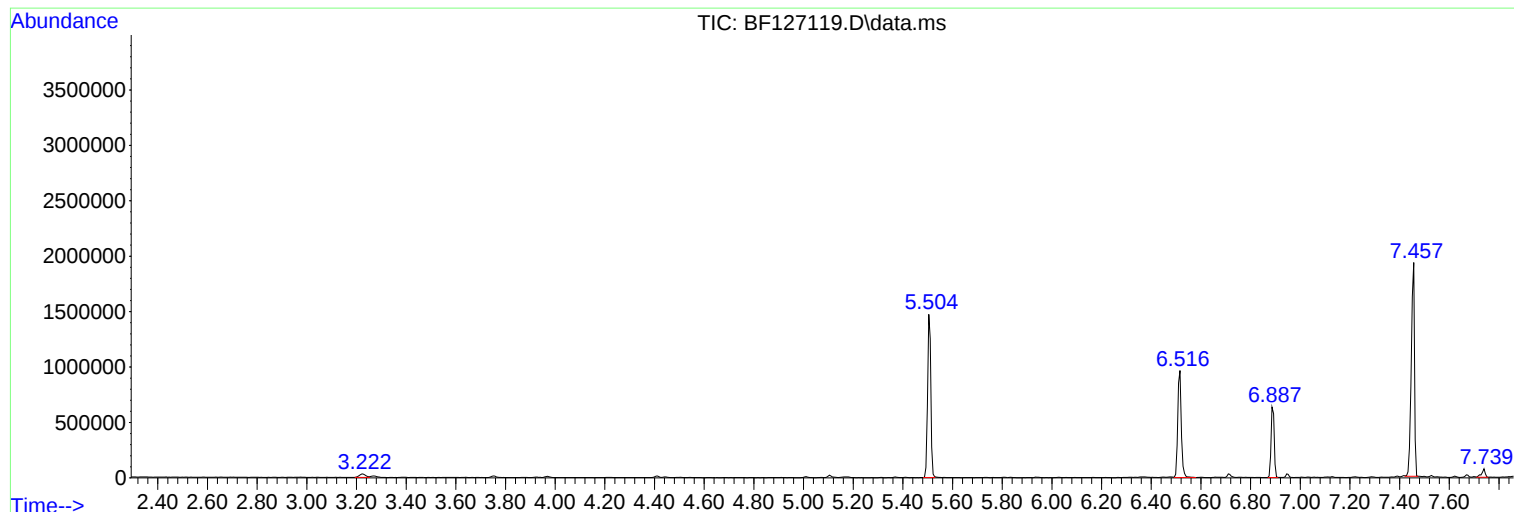
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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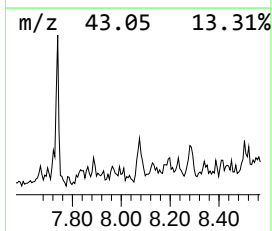
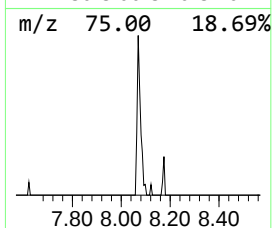
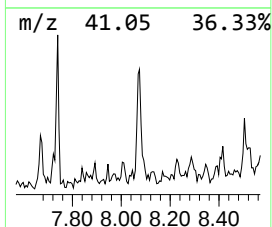
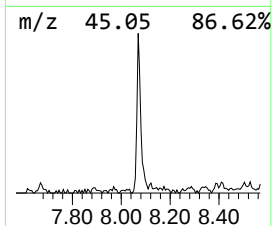
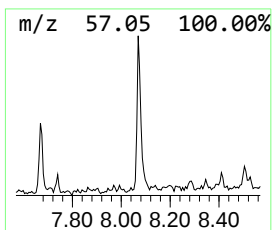
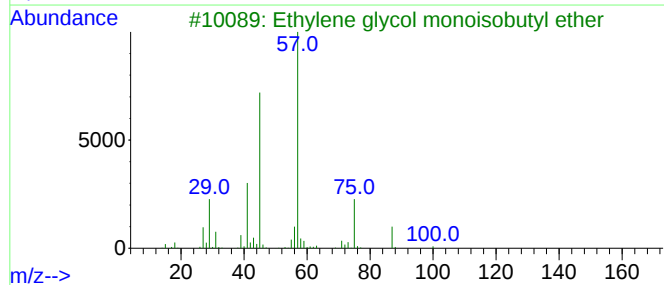
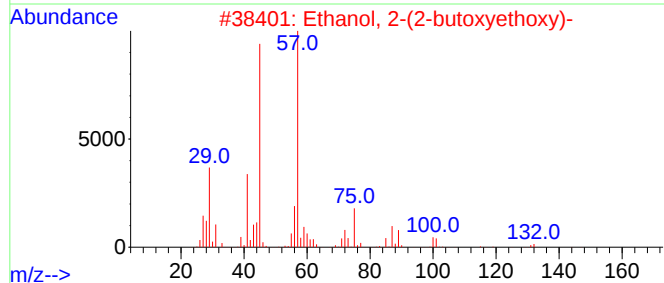
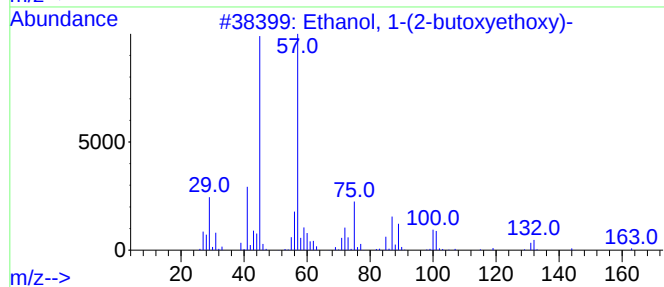
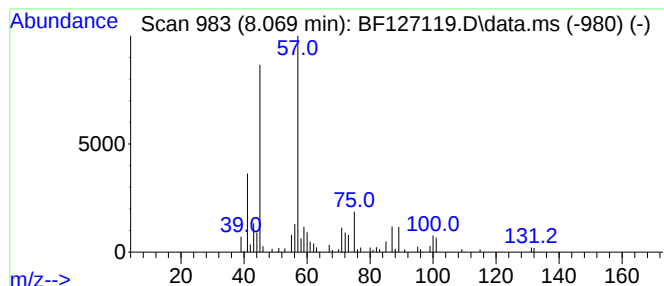
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.069	2.00 ng	73318	Naphthalene-d8	8.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	86
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	47
5			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	47



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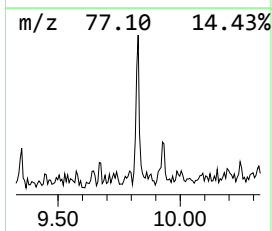
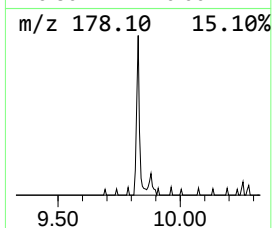
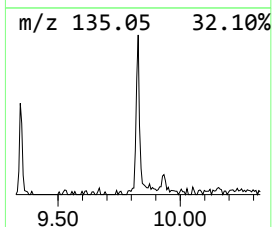
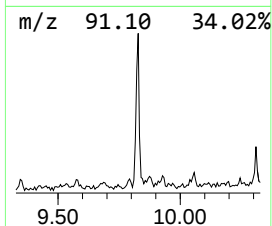
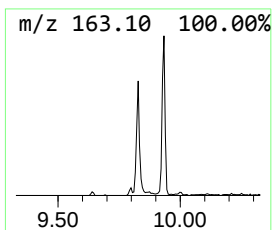
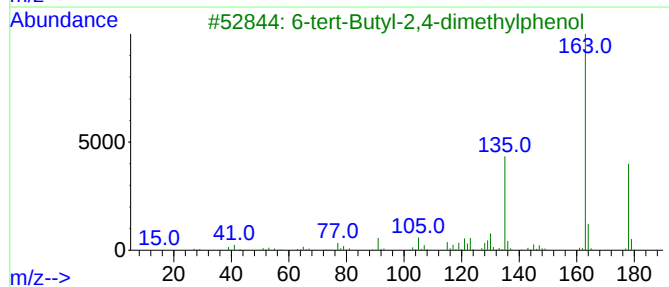
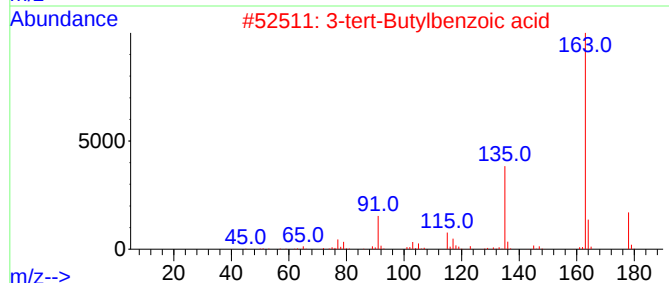
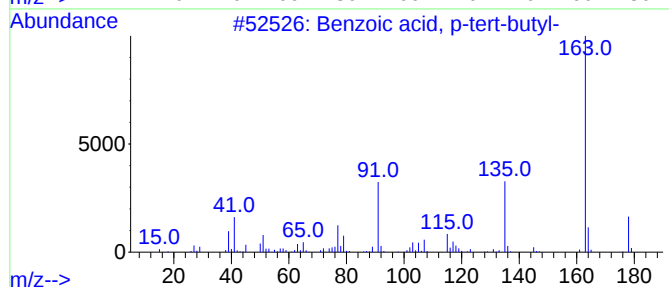
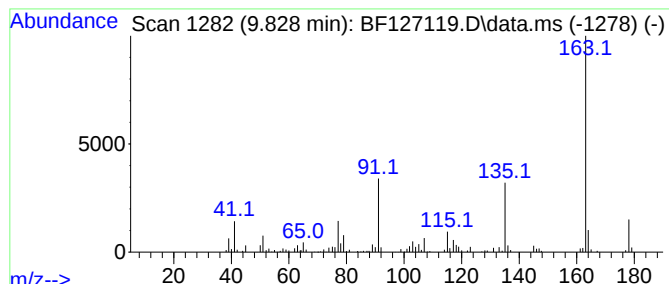
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzoic acid, p-tert-butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.828	2.49 ng	104127	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	96
2			3-tert-Butylbenzoic acid	178	C11H14O2	007498-54-6	90
3			6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	68
4			5-Fluoro-8-quinolinol	163	C9H6FN0	000387-97-3	59
5			3-pyridinecarbonitrile, 2-amino-...	163	C8H9N3O	1010404-44-3	58



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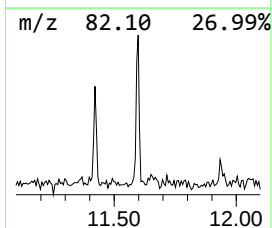
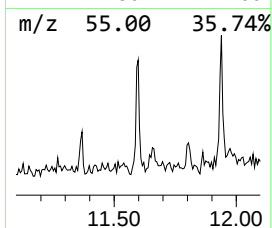
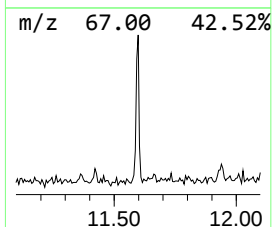
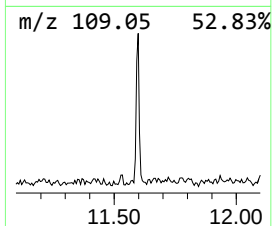
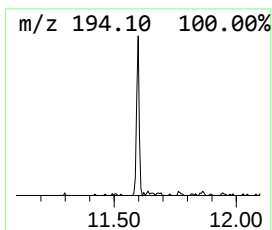
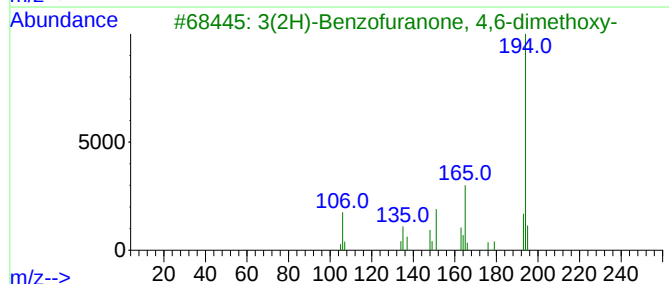
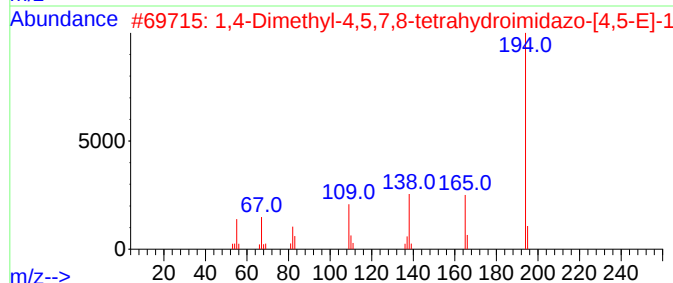
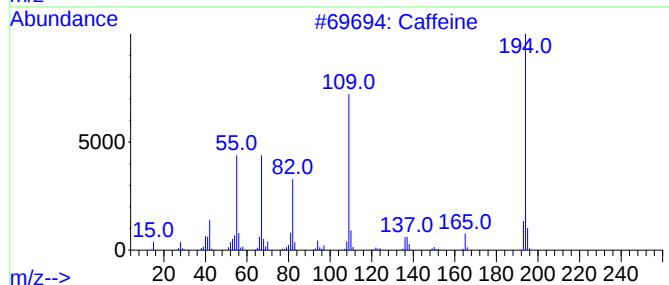
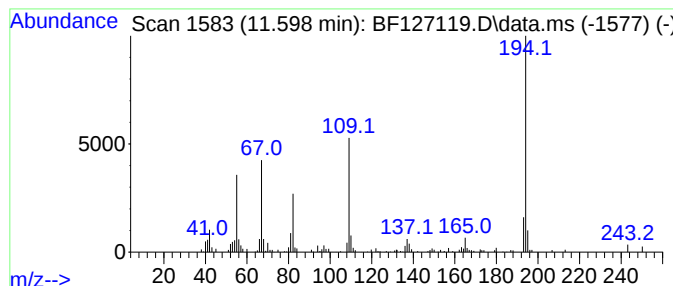
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Caffeine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.598	2.75 ng	115262	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Caffeine	194	C8H10N4O2	000058-08-2	95
2			1,4-Dimethyl-4,5,7,8-tetrahydroi...	194	C8H10N4O2	130063-15-9	64
3			3(2H)-Benzofuranone, 4,6-dimethoxy-	194	C10H10O4	004225-35-8	50
4			2-Fluorobenzylamine, N,N-dibutyl	237	C15H24FN	1000310-31-2	47
5			3,3'-Dimethyl-5-methoxy-4,5'-bii...	194	C9H10N2O3	019668-80-5	38



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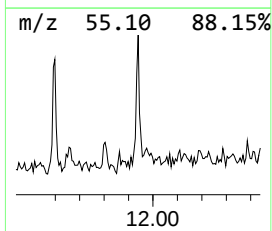
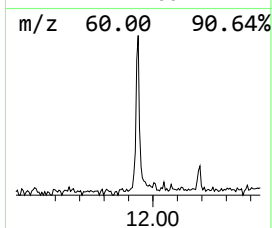
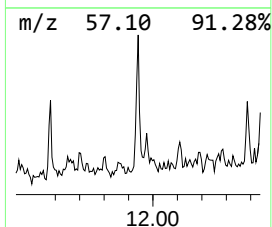
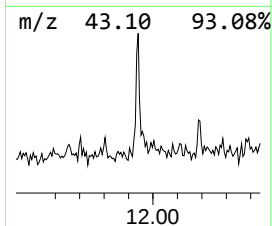
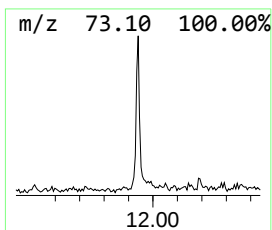
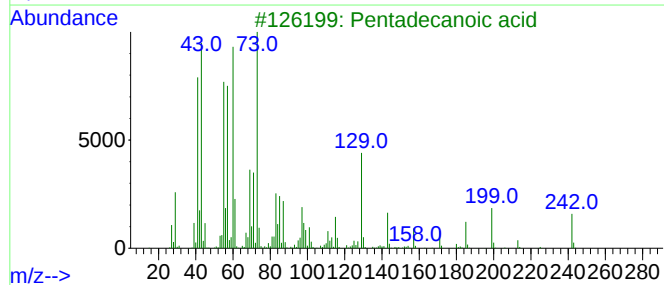
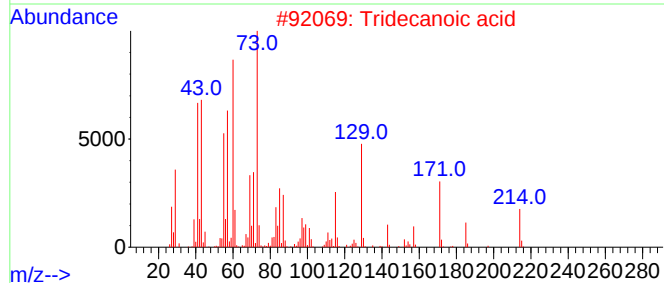
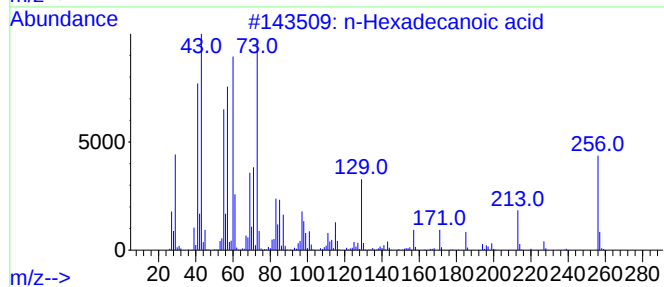
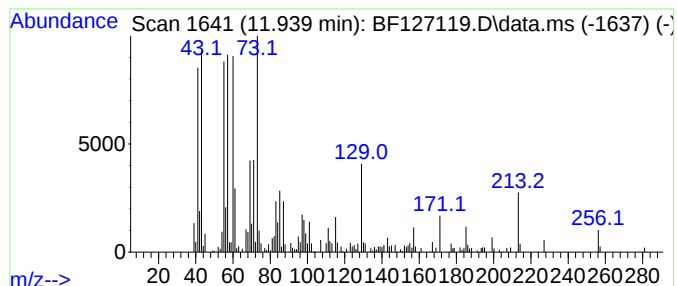
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.939	2.83 ng	118608	Phenanthrene-d10	11.422	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64



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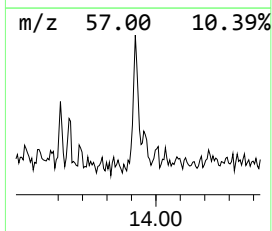
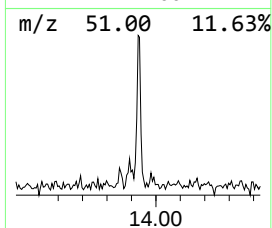
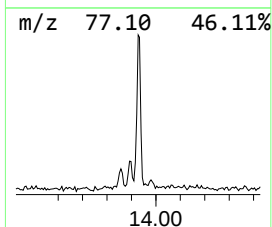
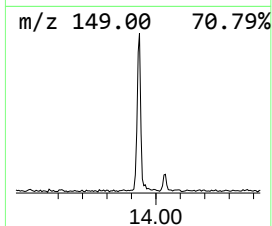
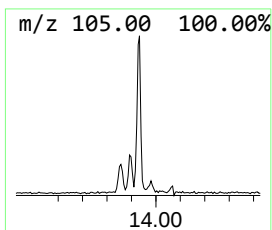
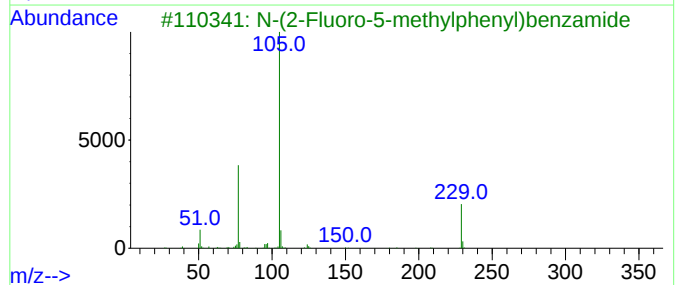
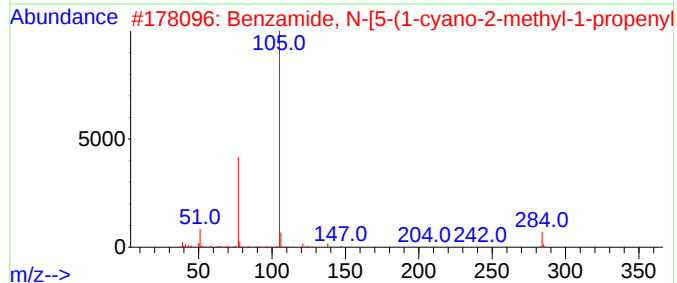
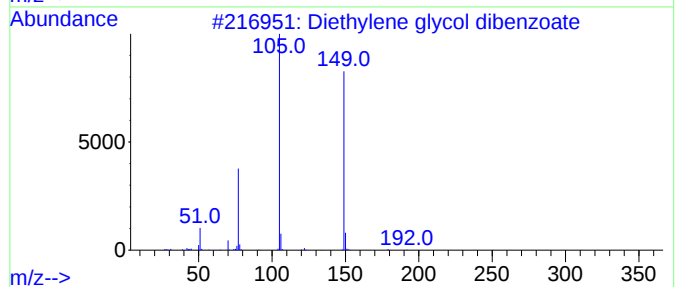
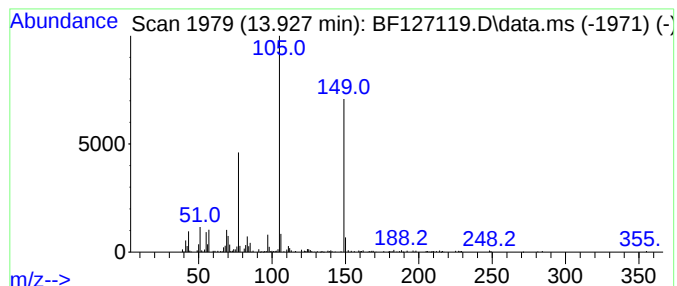
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Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	10.06 ng	244887	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	64
2			Benzamide, N-[5-(1-cyano-2-methy...	284	C14H12N4O5	172535-11-4	43
3			N-(2-Fluoro-5-methylphenyl)benza...	229	C14H12FNO	143925-45-5	43
4			N,N-Bis(2-cyanoethyl)benzamide	227	C13H13N3O	003232-12-0	43
5			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 1-(2-b...	8.069	2.0	ng	73318	2	8.175	731434	20.0
Benzoic acid, p...	9.828	2.5	ng	104127	3	9.933	834786	20.0
Caffeine	11.598	2.8	ng	115262	4	11.422	839378	20.0
n-Hexadecanoic ...	11.939	2.8	ng	118608	4	11.422	839378	20.0
Diethylene glyc...	13.927	10.1	ng	244887	5	14.068	486726	20.0