LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090821\
Data File : BF125398.D
Acq On : 8 Sep 2021 13:11
Operator : JU/CG
Sample : PB138943BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB138943BL

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125398.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.240	16	26	33	rVB	118675	167840	2.63%	0.438%
2	5.522	578	584	587	rBV	4892090	5056742	79.34%	13.183%
3	6.522	748	754	757	rBV	4079008	4983862	78.20%	12.993%
4	6.886	812	816	819	rBV	1196414	1029052	16.15%	2.683%
5	7.451	906	912	915	rBV	3190047	3345355	52.49%	8.721%
6	8.169	1029	1034	1037	rBV	1520659	1364555	21.41%	3.557%
7	9.245	1211	1217	1220	rBV	5683627	5801802	91.03%	15.125%
8	9.922	1327	1332	1336	rBV	1626252	1563741	24.54%	4.077%
9	10.716	1462	1467	1471	rBV	3786697	3865883	60.66%	10.078%
10	11.416	1581	1586	1589	rBV	1794277	1661807	26.07%	4.332%
11	13.004	1851	1856	1859	rBV	6464456	6373315	100.00%	16.615%
12	13.845	1991	1999	2002	rBV	88887	127753	2.00%	0.333%
13	13.886	2002	2006	2008	rVV	122344	153640	2.41%	0.401%
14	13.921	2008	2012	2017	rVB	362476	398445	6.25%	1.039%
15	14.057	2031	2035	2038	rBV	1387842	1240329	19.46%	3.233%
16	15.545	2283	2288	2298	rVB	861071	1047533	16.44%	2.731%
17	17.162	2552	2563	2576	rVB7	38596	177719	2.79%	0.463%

Sum of corrected areas: 38359373

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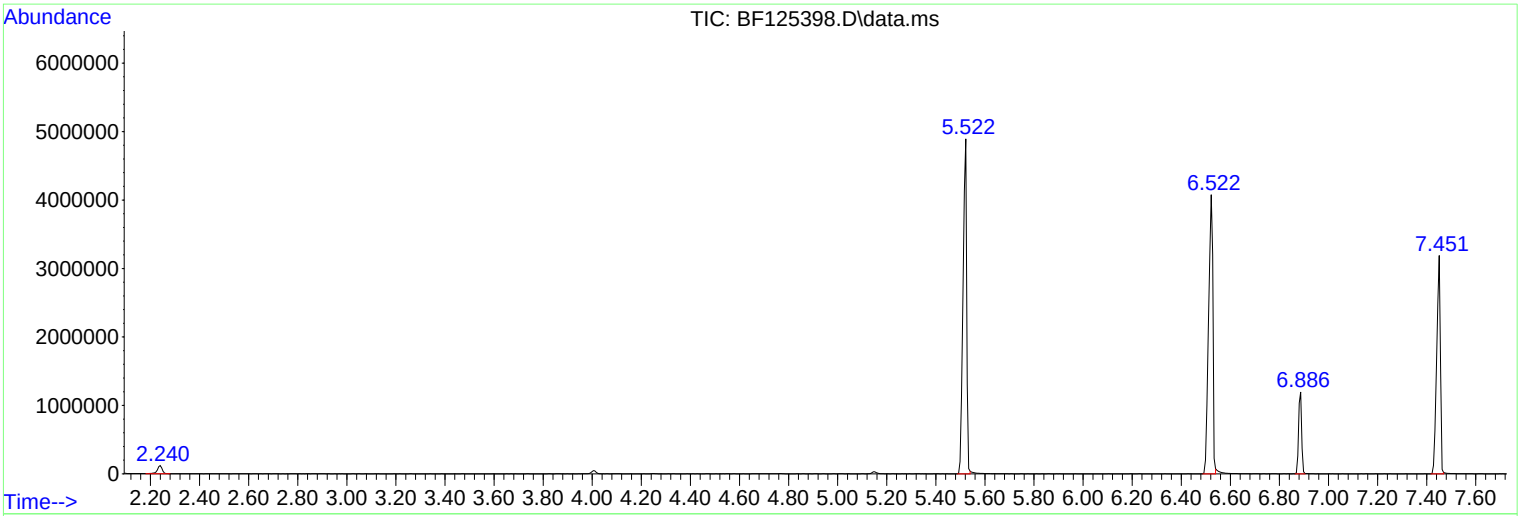
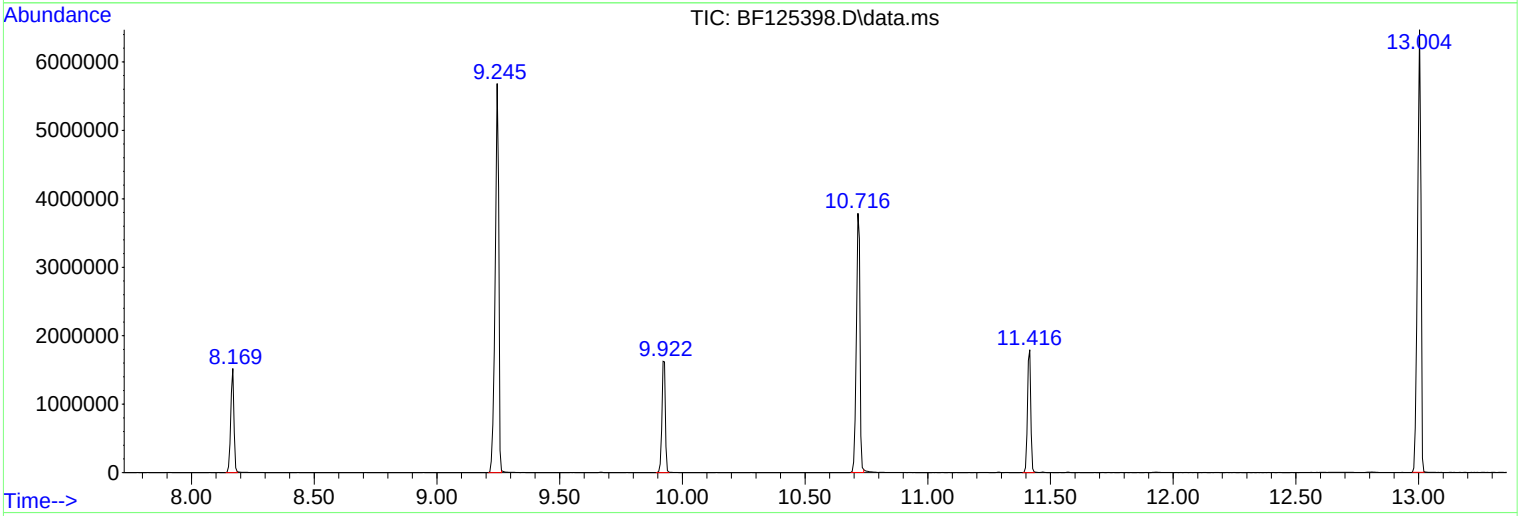
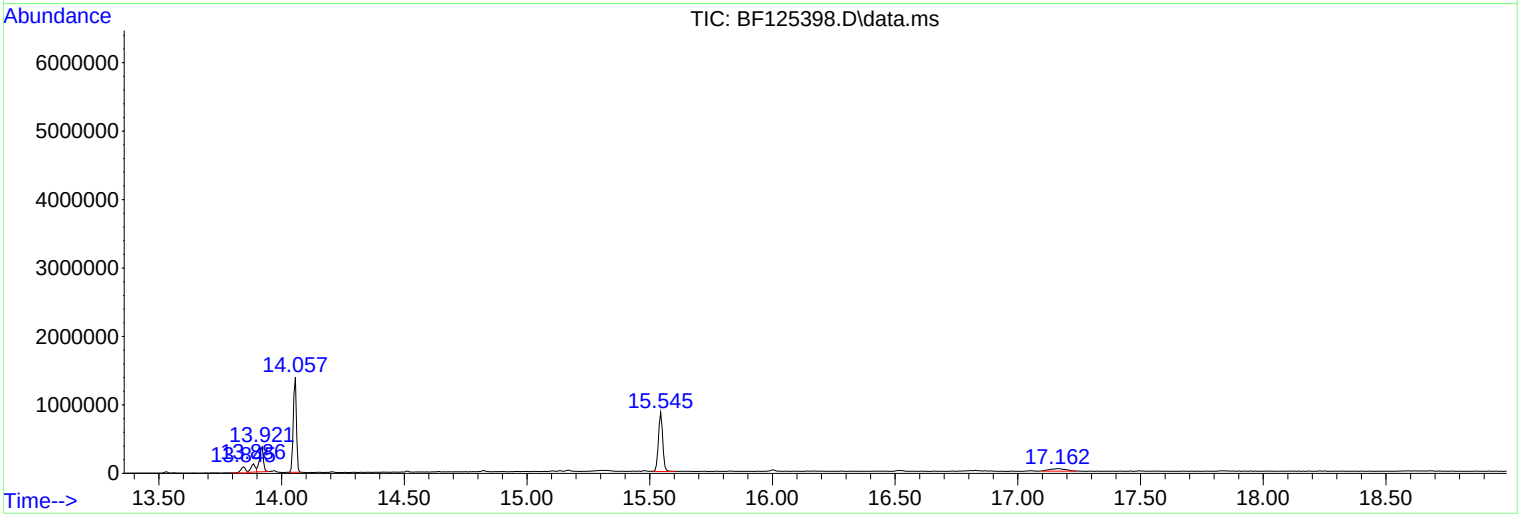
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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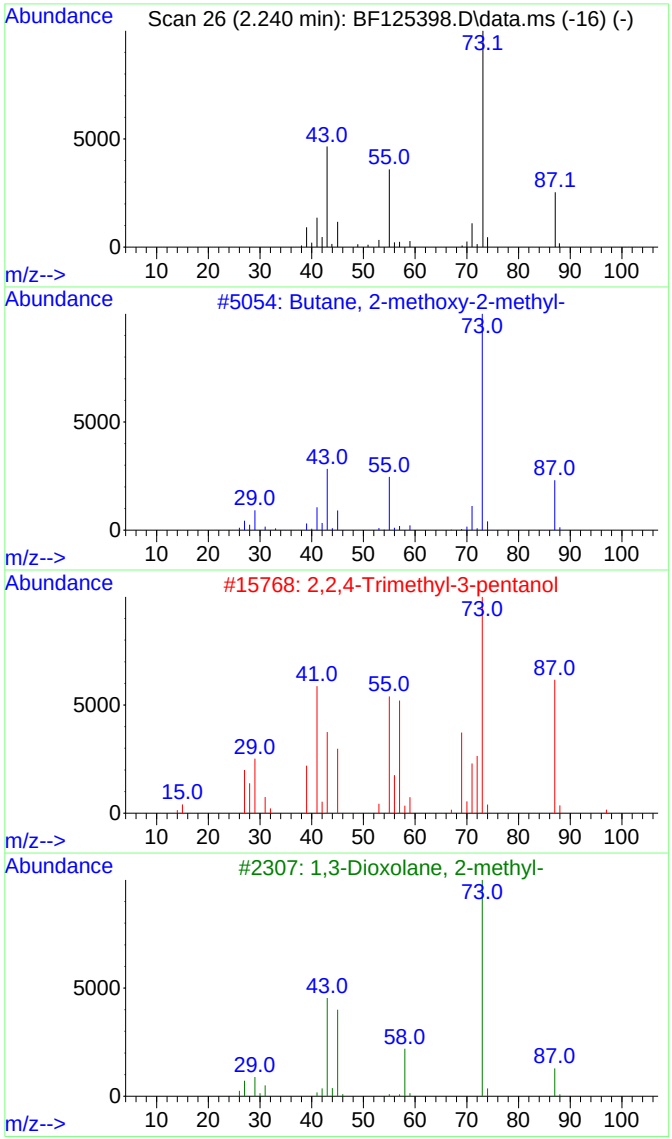
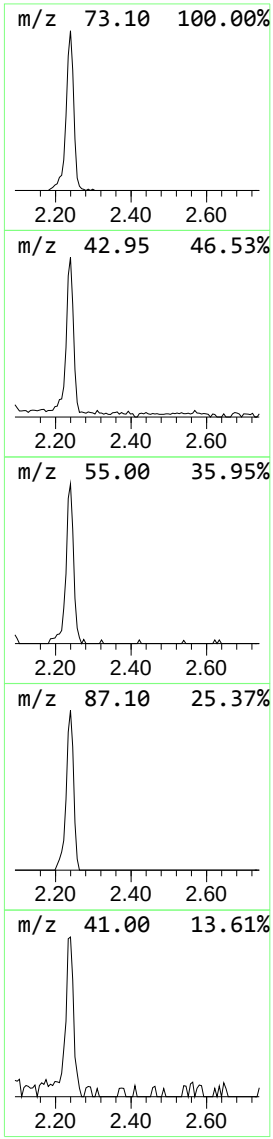
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.240	3.26 ng	167840	1,4-Dichlorobenzene-d4	6.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23





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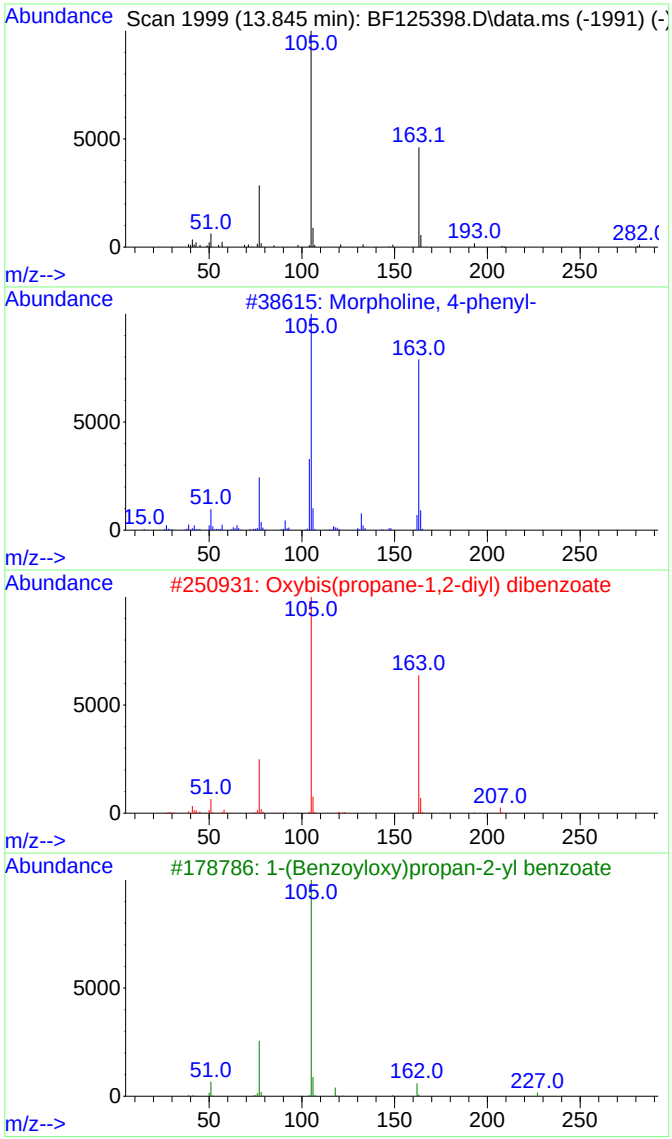
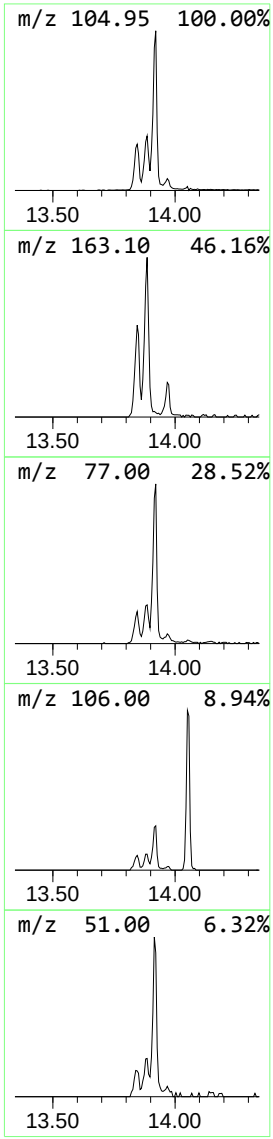
Peak Number 2 Morpholine, 4-phenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	2.06 ng	127753	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	80
2	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	64
3	1-(Benzoyloxy)propan-2-yl benzoate	284	C17H16O4	019224-26-1	35
4	Benzoic acid, 2-propenyl ester	162	C10H10O2	000583-04-0	27
5	(5-tert-Butyl-2-hydroxyphenyl)(p...	254	C17H18O2	1000468-68-2	27





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Instrument : BNA_F
ClientSampleId : PB138943BL

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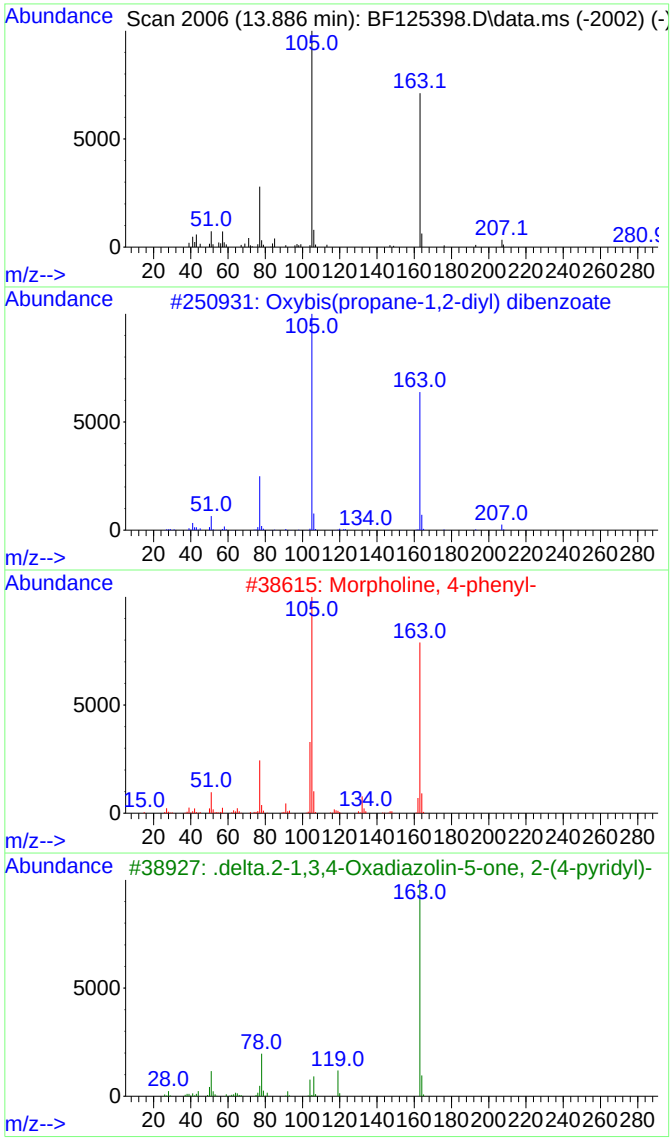
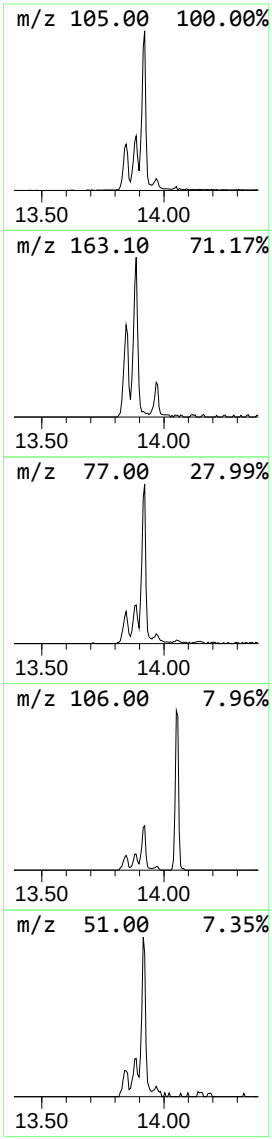
Peak Number 3 Oxybis(propane-1,2-diyl) di... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	2.48 ng	153640	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	72
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	52
3	.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	38
4	Diethyl benzamidomalonate	279	C14H17NO5	016798-45-1	35
5	Butanedioic acid, 2,3-bis(benzoy...	358	C18H14O8	017026-42-5	27





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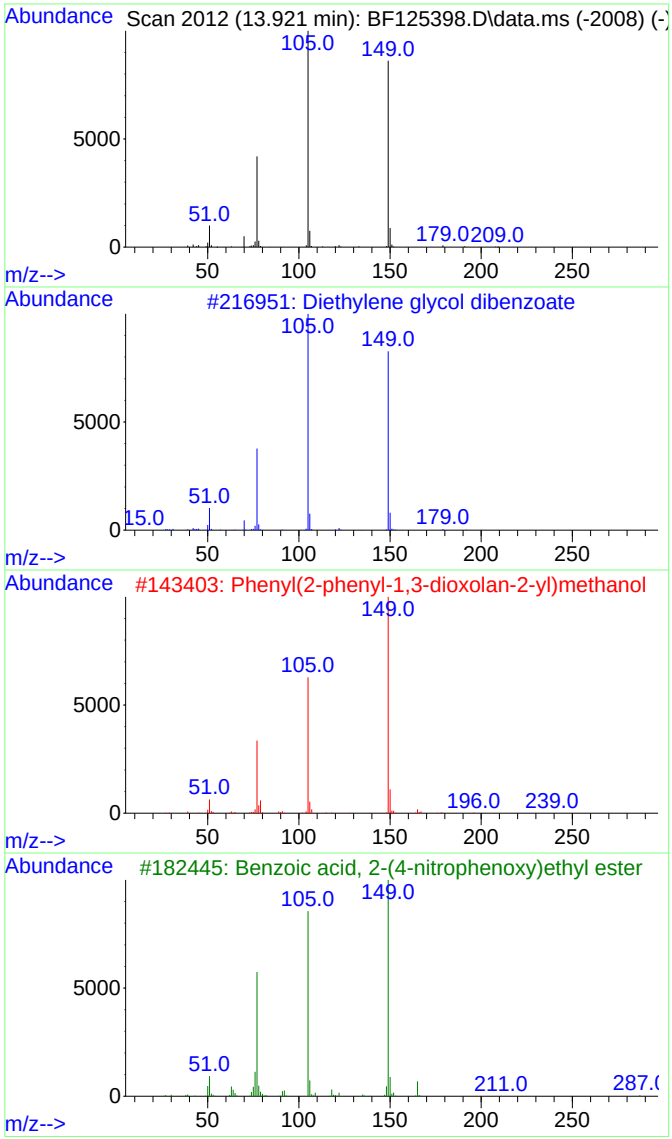
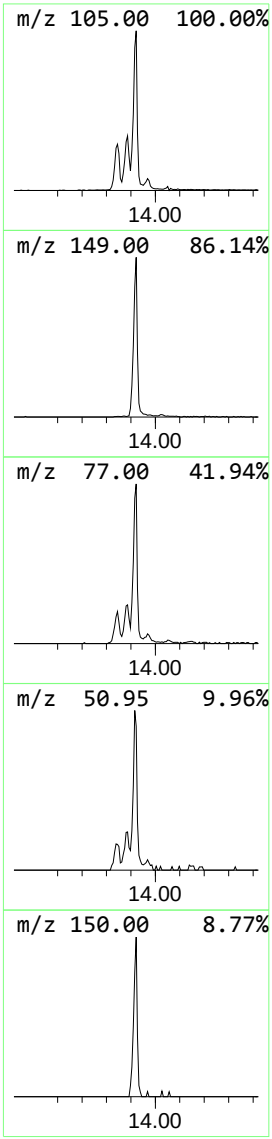
Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	6.42 ng	398445	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	91
2	Phenyl(2-phenyl-1,3-dioxolan-2-y...	256	C16H16O3	005694-69-9	78
3	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	72
4	Benzoic acid, 2-(2-chlorophenoxy...	276	C15H13ClO3	1000368-25-9	72
5	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	52





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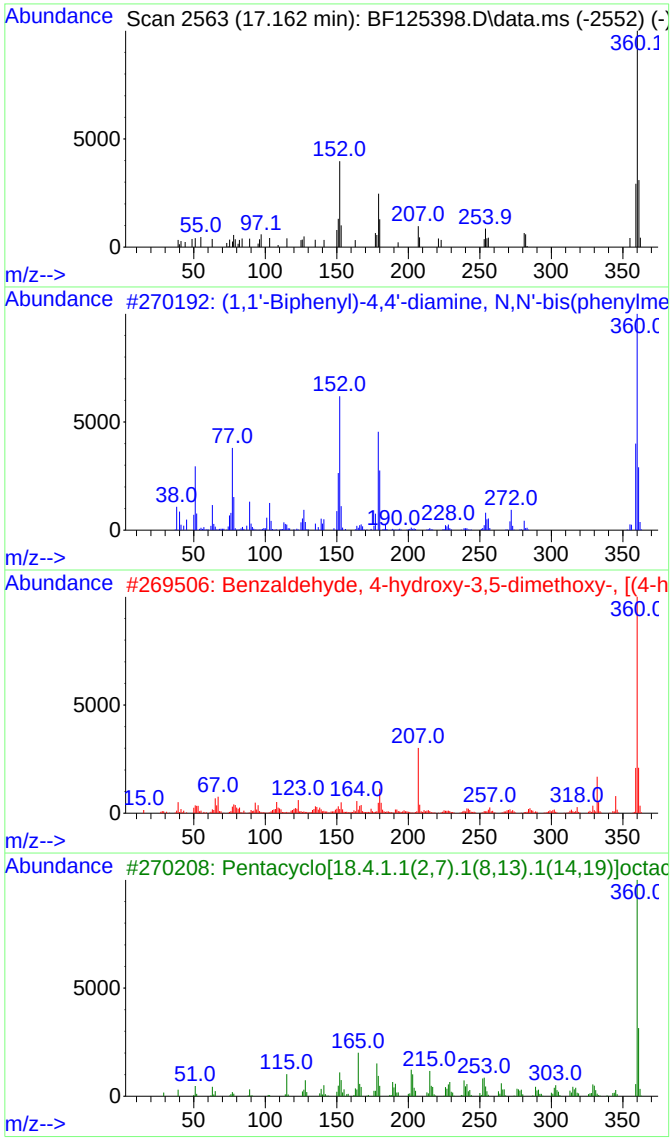
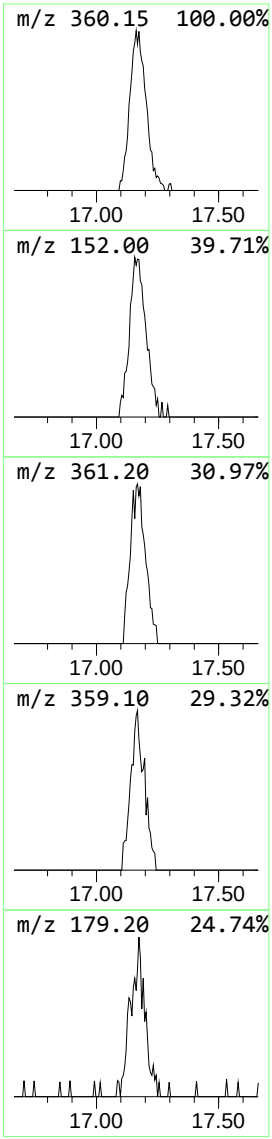
****
Peak Number 5 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.162	3.39 ng	177719	Perylene-d12	15.545

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1,1'-Biphenyl)-4,4'-diamine, N,...	360	C26H20N2	006311-48-4	93
2	Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	49
3	Pentacyclo[18.4.1.1(2,7).1(8,13)...	360	C28H24	101077-60-5	47
4	1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13BO6	1000150-23-7	47
5	7H-[1,2,4]Triazolo[3,4-b][1,3,4]...	360	C16H10F2N4S2	1000310-22-0	47





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.240	3.3	ng	167840	1	6.886	1029050	20.0
Morpholine, 4-p...	13.845	2.1	ng	127753	5	14.057	1240330	20.0
Oxybis(propane-...	13.886	2.5	ng	153640	5	14.057	1240330	20.0
Diethylene glyc...	13.921	6.4	ng	398445	5	14.057	1240330	20.0
(1,1'-Biphenyl)...	17.162	3.4	ng	177719	6	15.545	1047530	20.0