

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
 Data File : BF125206.D
 Acq On : 25 Aug 2021 13:11
 Operator : JU/CG
 Sample : M3524-06
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PE-6

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: BF125206.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	15	21	29	rVB	812853	1082964	32.10%	4.316%
2	5.534	581	586	589	rBV	2978024	2920312	86.57%	11.638%
3	6.534	751	756	759	rBV	3051204	2914928	86.41%	11.617%
4	6.916	817	821	824	rBV	971327	869562	25.78%	3.465%
5	7.475	911	916	919	rBV	2209118	1911767	56.67%	7.619%
6	8.098	1018	1022	1035	rBV2	63354	154009	4.57%	0.614%
7	8.198	1035	1039	1042	rBV	1296174	1120887	33.23%	4.467%
8	9.269	1217	1221	1224	rBV	3943516	3373526	100.00%	13.444%
9	9.951	1333	1337	1340	rBV	1556621	1262423	37.42%	5.031%
10	10.739	1467	1471	1474	rBV	2449028	2204465	65.35%	8.785%
11	11.439	1586	1590	1597	rBV	1509524	1276398	37.84%	5.087%
12	11.957	1674	1678	1683	rBV	209313	195293	5.79%	0.778%
13	12.745	1808	1812	1824	rVB	65555	91314	2.71%	0.364%
14	13.021	1855	1859	1863	rBV	3428953	3349543	99.29%	13.349%
15	13.874	1999	2004	2007	rBV	33879	48320	1.43%	0.193%
16	13.910	2007	2010	2013	rVV	50839	52058	1.54%	0.207%
17	13.945	2013	2016	2019	rVV	130637	133281	3.95%	0.531%
18	13.992	2019	2024	2035	rVV8	58635	218487	6.48%	0.871%
19	14.080	2035	2039	2042	rVB	986104	919713	27.26%	3.665%
20	14.857	2166	2171	2178	rBV5	24856	44608	1.32%	0.178%
21	15.574	2288	2293	2305	rVB2	688400	907740	26.91%	3.618%
22	16.051	2370	2374	2380	rVB	29353	40701	1.21%	0.162%

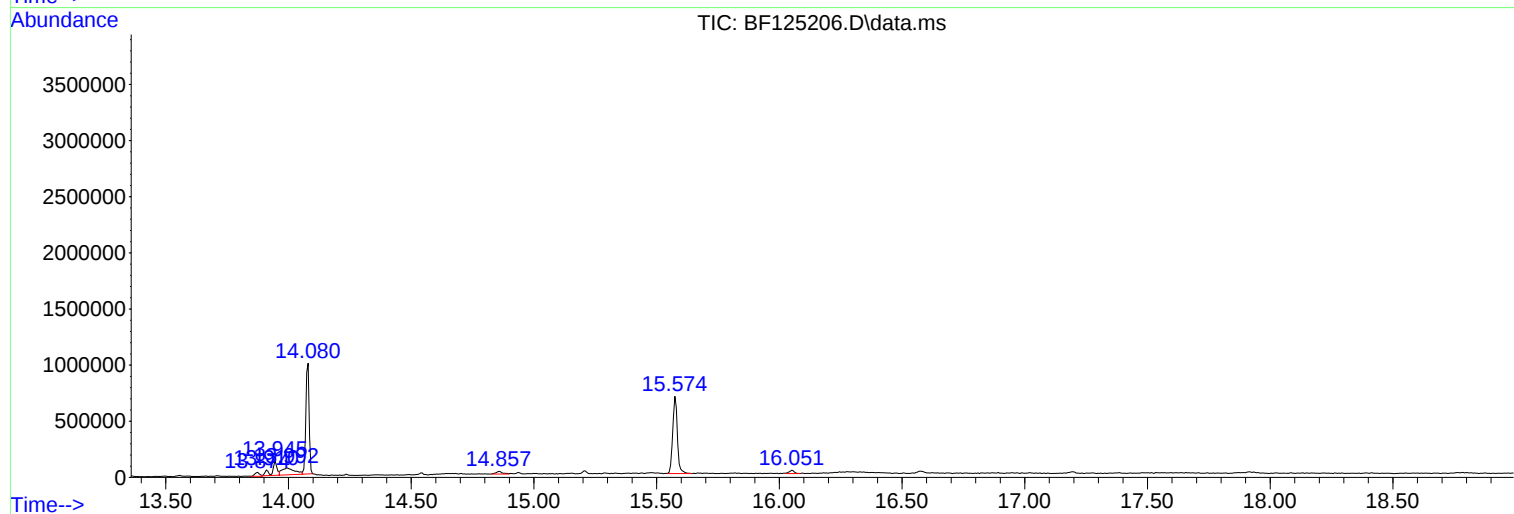
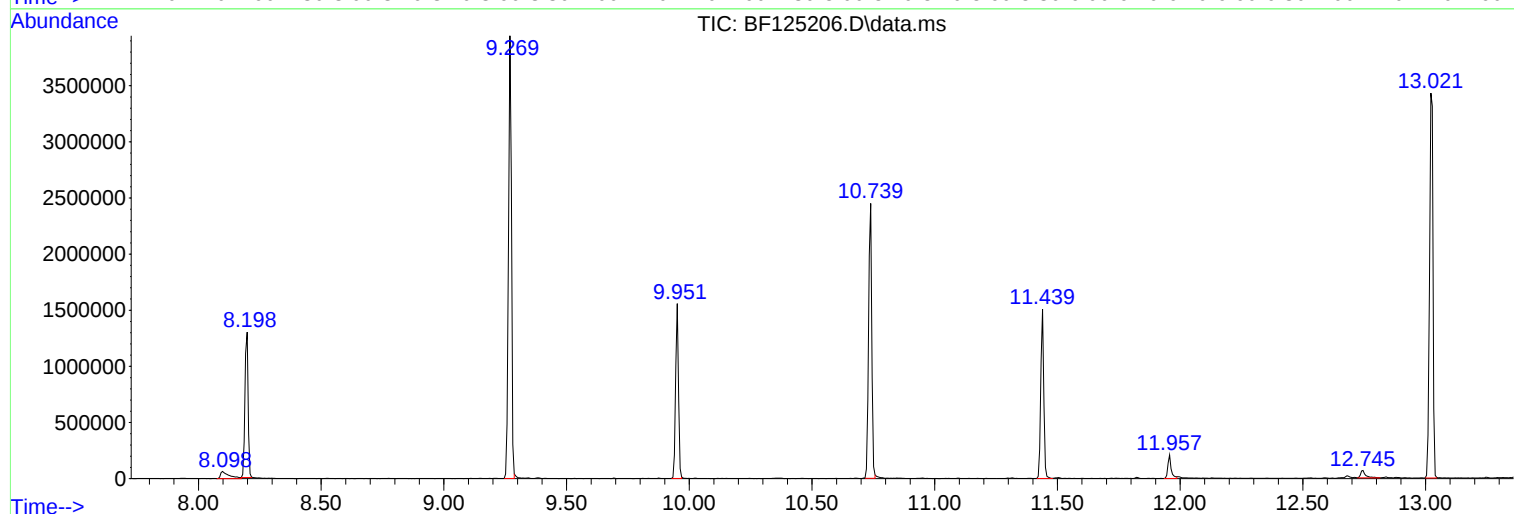
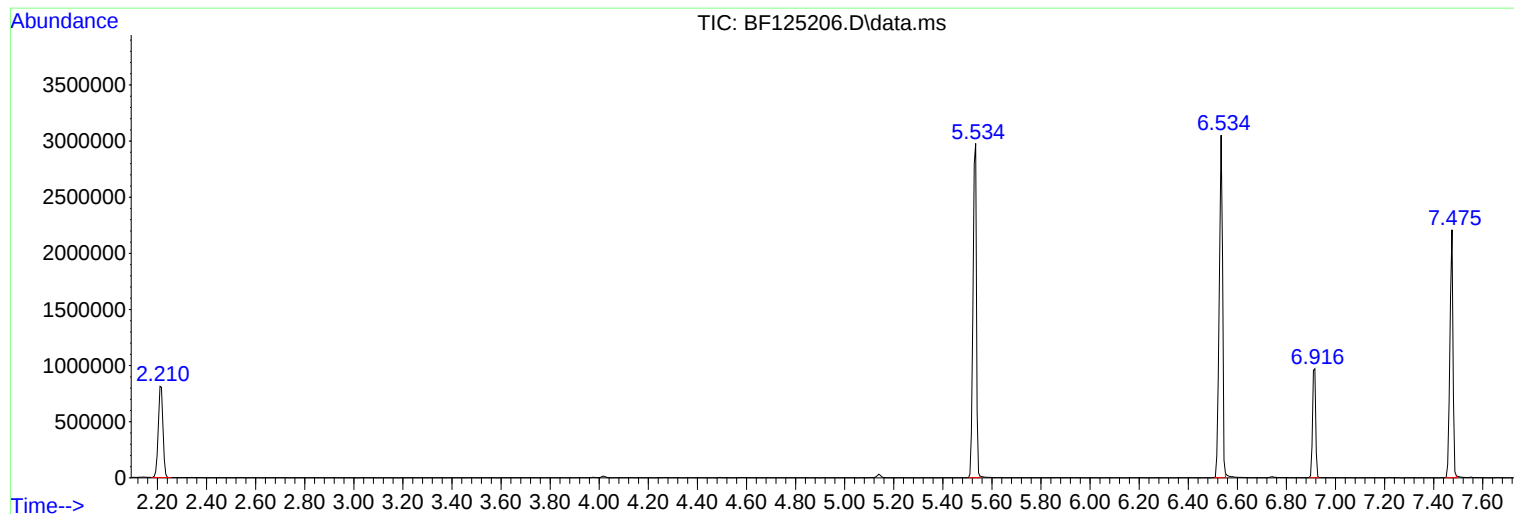
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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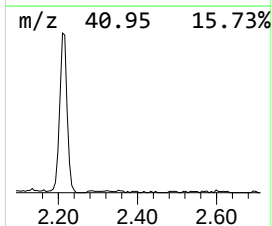
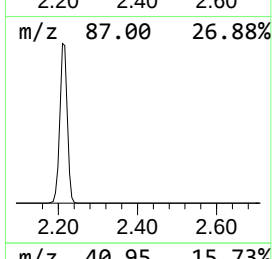
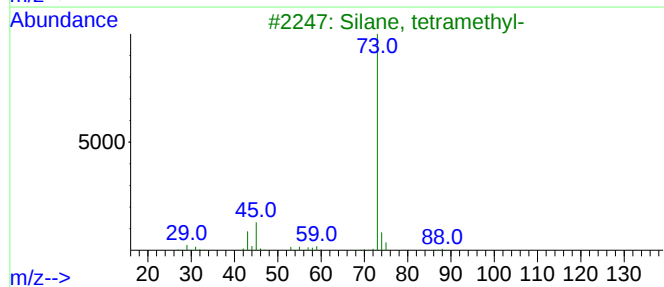
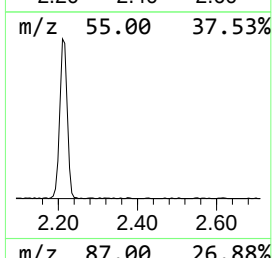
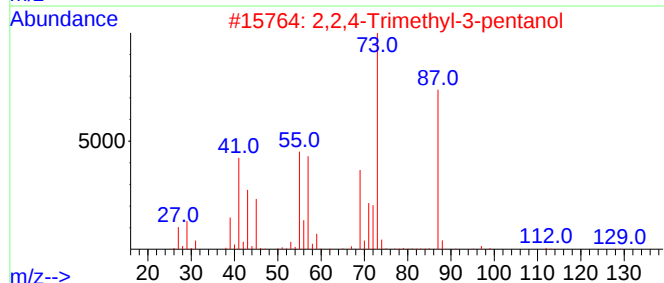
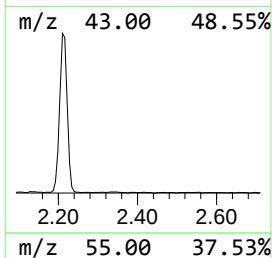
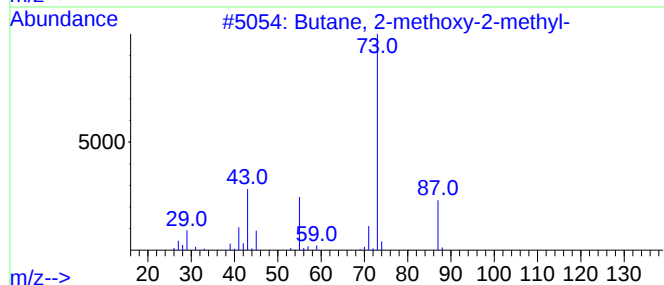
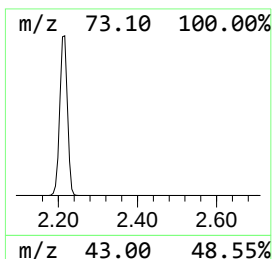
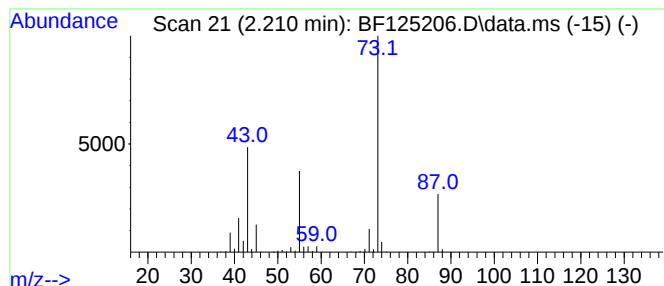
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.210	24.91 ng	1082960	1,4-Dichlorobenzene-d4	6.916

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	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25



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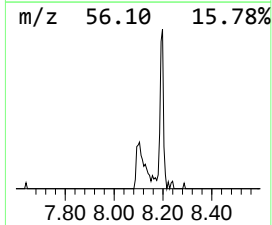
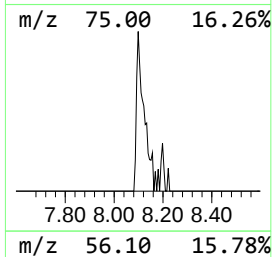
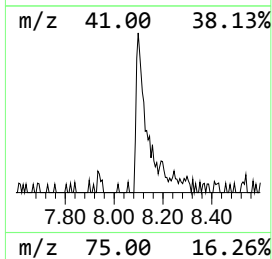
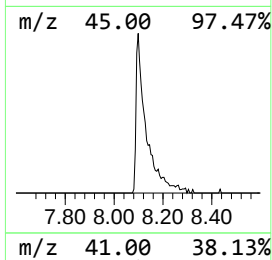
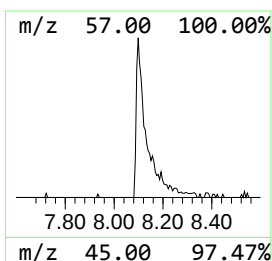
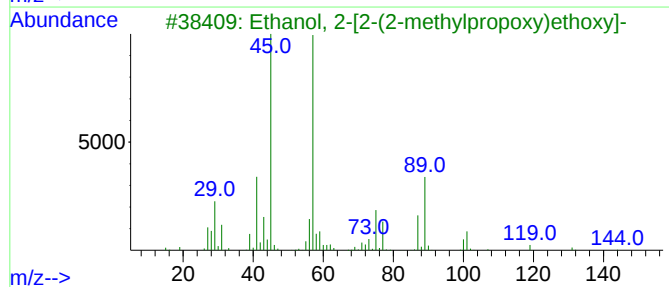
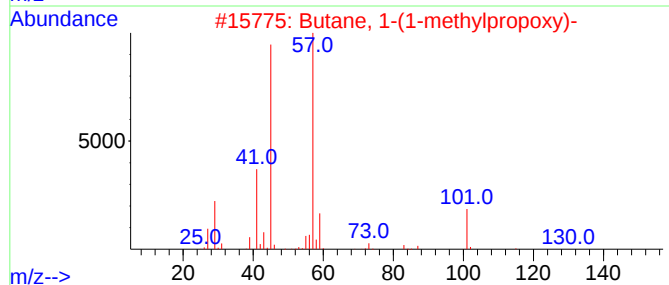
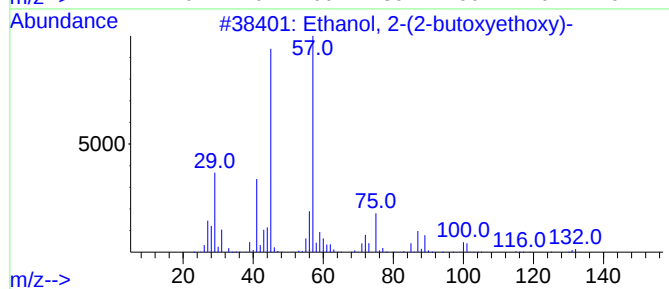
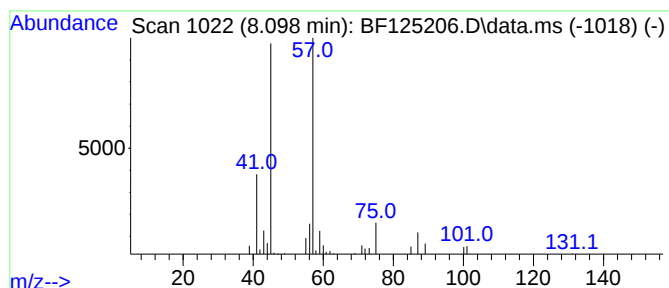
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	2.75 ng	154009	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	74
2			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	59
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	45



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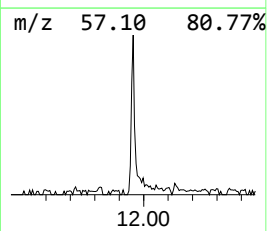
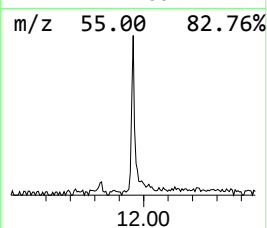
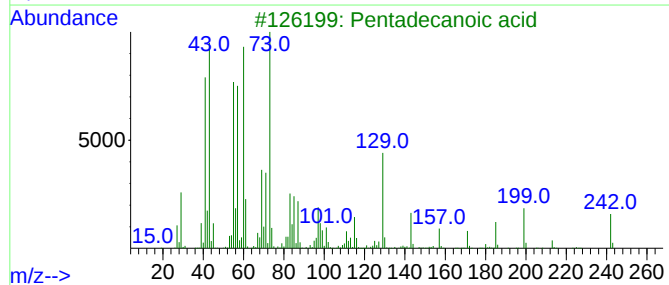
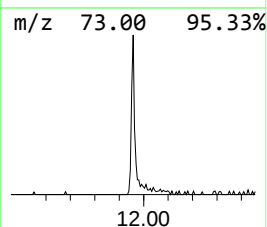
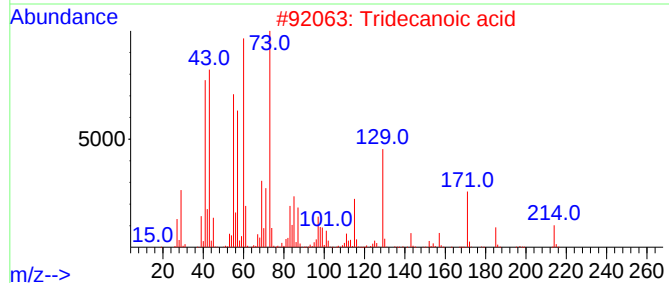
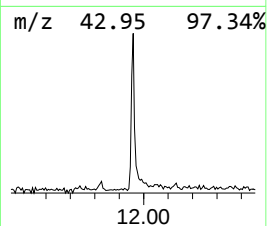
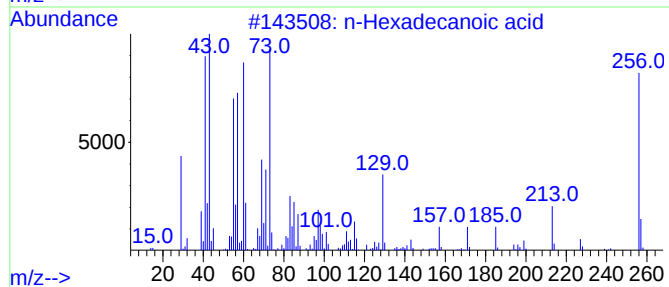
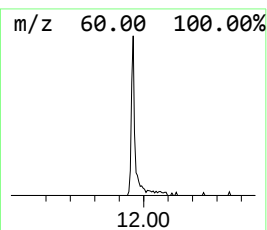
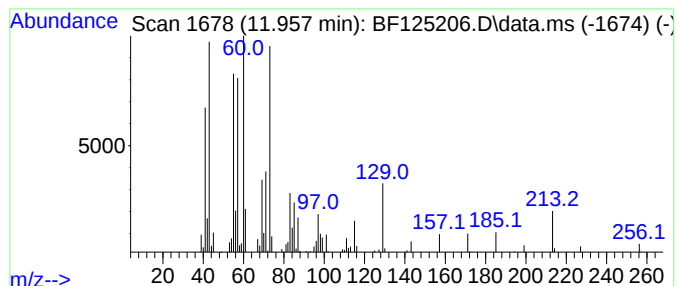
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	3.06 ng	195293	Phenanthrene-d10	11.439

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	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	72



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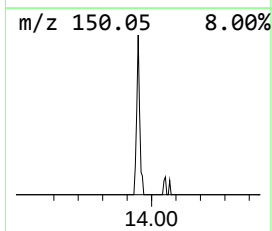
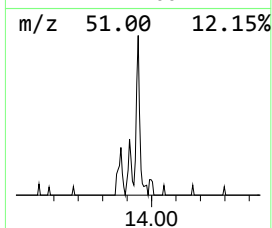
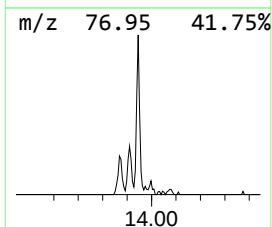
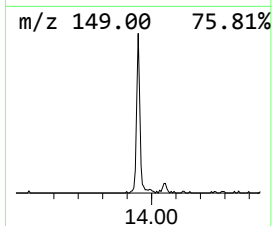
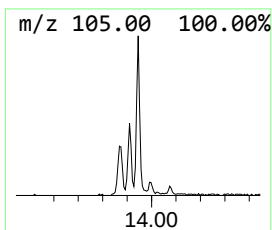
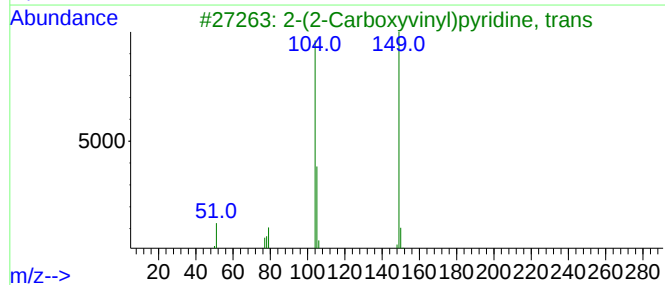
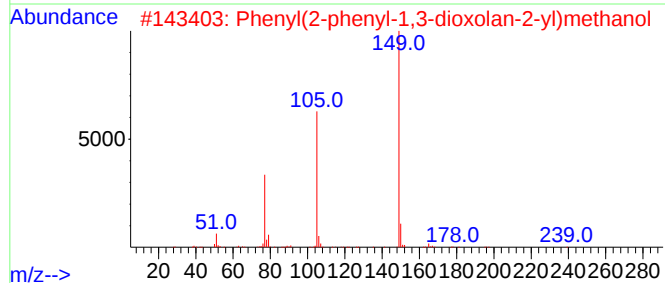
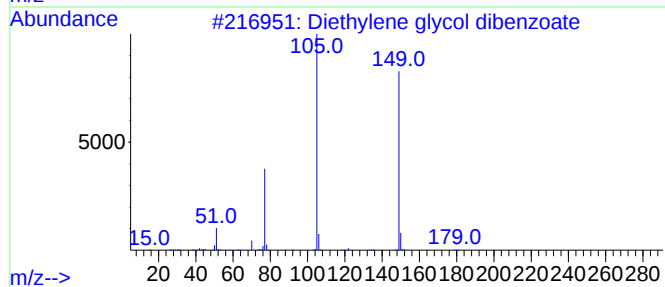
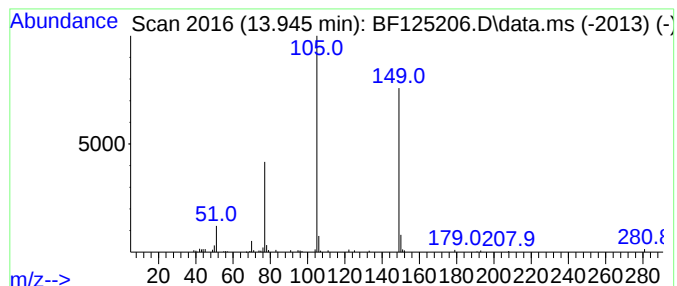
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Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	2.90 ng	133281	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2			Phenyl(2-phenyl-1,3-dioxolan-2-yl)methanol	256	C16H16O3	005694-69-9	64
3			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	59
4			2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	43
5			N-Benzoyl-L-beta.-alanine	193	C10H11NO3	003440-28-6	38



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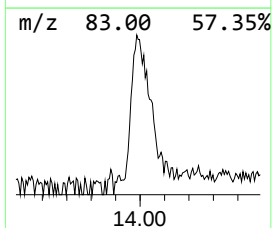
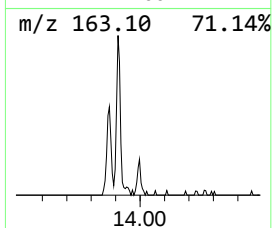
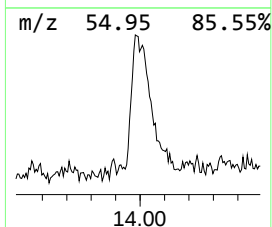
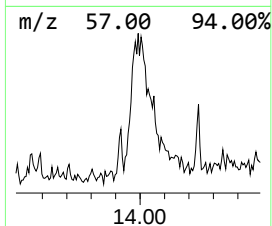
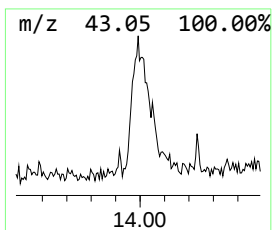
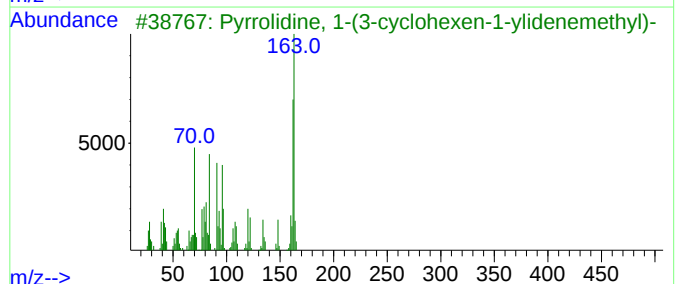
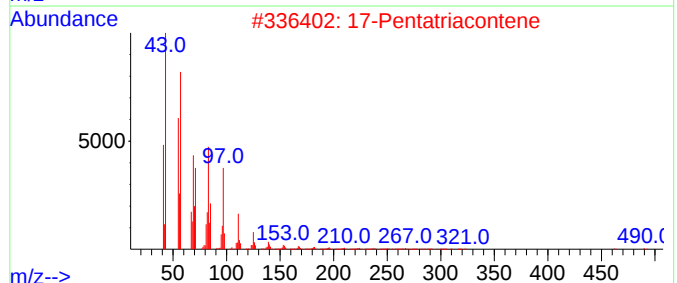
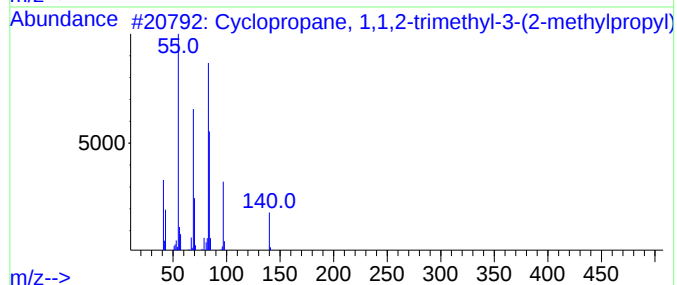
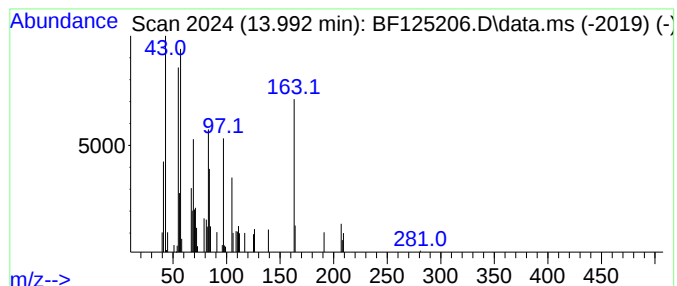
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown13.992 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.992	4.75 ng	218487	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,1,2-trimethyl-3-...	140	C10H20	041977-43-9	35
2			17-Pentatriacontene	491	C35H70	006971-40-0	35
3			Pyrrolidine, 1-(3-cyclohexen-1-y...	163	C11H17N	018205-60-2	35
4			1-Dodecanol, 2-octyl-, acetate	340	C22H44O2	074051-84-6	35
5			1,3-Cyclohexanedione, 5-isopropyl-	154	C9H14O2	018456-87-6	35



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.210	24.9	ng	1082960	1	6.916	869562	20.0
Ethanol, 2-(2-b...	8.098	2.8	ng	154009	2	8.198	1120890	20.0
n-Hexadecanoic ...	11.957	3.1	ng	195293	4	11.439	1276400	20.0
Diethylene glyc...	13.945	2.9	ng	133281	5	14.080	919713	20.0
unknown13.992	13.992	4.8	ng	218487	5	14.080	919713	20.0