

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051525\
 Data File : BF142408.D
 Acq On : 15 May 2025 23:01
 Operator : RC/JU
 Sample : Q1982-05
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-5

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-BF050525.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142408.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.116	488	497	508	rBV	194432	290764	9.35%	1.308%
2	5.516	558	565	570	rBV	1851718	2535472	81.53%	11.403%
3	6.522	729	736	741	rBV	1873611	2604418	83.75%	11.713%
4	6.898	795	800	805	rBV	721398	890517	28.64%	4.005%
5	7.457	889	895	900	rBV	1255996	1652539	53.14%	7.432%
6	7.710	934	938	944	rVB	29006	36138	1.16%	0.163%
7	8.181	1013	1018	1035	rVB	933160	1182586	38.03%	5.318%
8	9.257	1195	1201	1206	rBV	2507656	3109853	100.00%	13.986%
9	9.939	1311	1317	1328	rBV	1001367	1308653	42.08%	5.885%
10	10.251	1362	1370	1381	rBV2	21068	69257	2.23%	0.311%
11	10.339	1381	1385	1397	rVB3	18761	38769	1.25%	0.174%
12	10.645	1432	1437	1445	rVB	131039	172991	5.56%	0.778%
13	10.722	1445	1450	1464	rBV	1392771	1774683	57.07%	7.981%
14	11.422	1564	1569	1577	rBV	918007	1182172	38.01%	5.317%
15	11.945	1653	1658	1670	rBV2	177707	302276	9.72%	1.359%
16	12.633	1771	1775	1780	rBV	44859	59696	1.92%	0.268%
17	12.733	1788	1792	1798	rBV6	18499	33342	1.07%	0.150%
18	12.863	1810	1814	1820	rBV	43693	64478	2.07%	0.290%
19	13.010	1833	1839	1844	rBV	1928713	2443036	78.56%	10.987%
20	13.774	1959	1969	1986	rVB7	137738	642137	20.65%	2.888%
21	13.904	1987	1991	2002	rBV	77313	154260	4.96%	0.694%
22	14.063	2013	2018	2030	rVB	739158	973350	31.30%	4.377%
23	15.551	2266	2271	2284	rVB	428011	714259	22.97%	3.212%

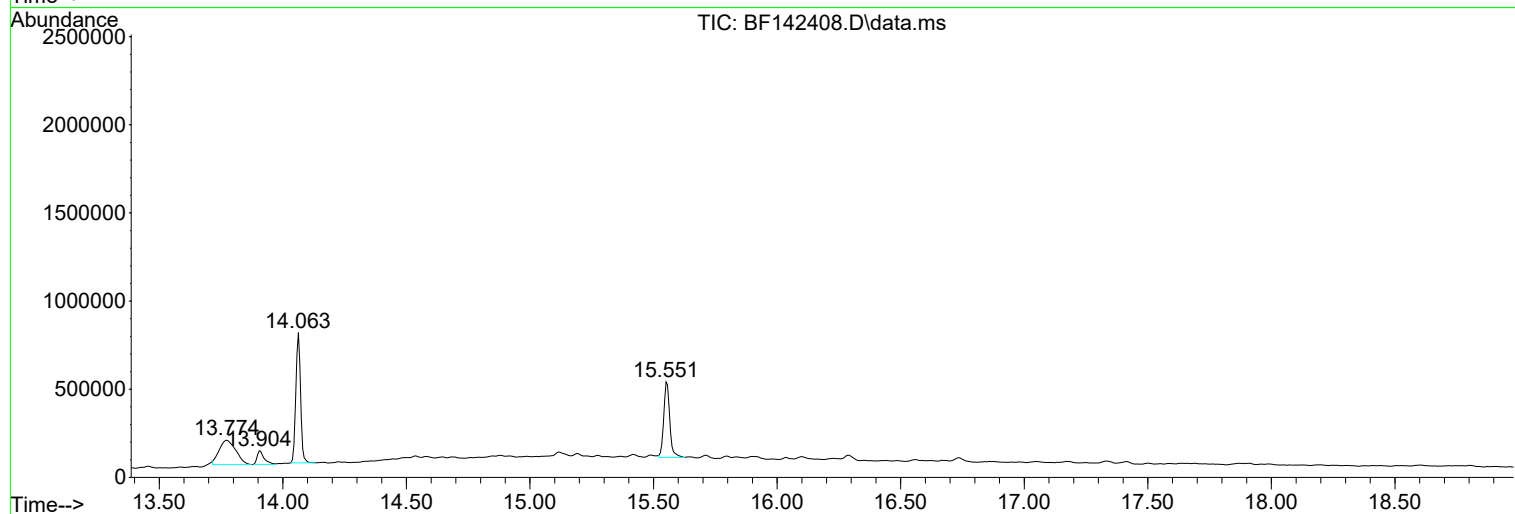
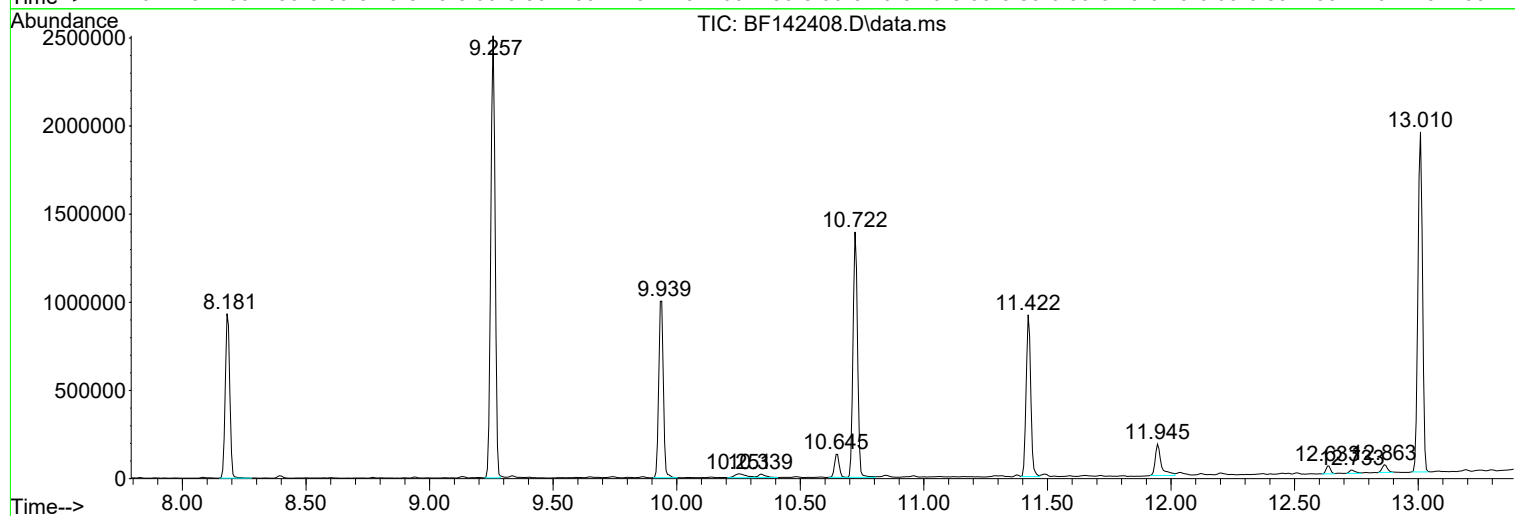
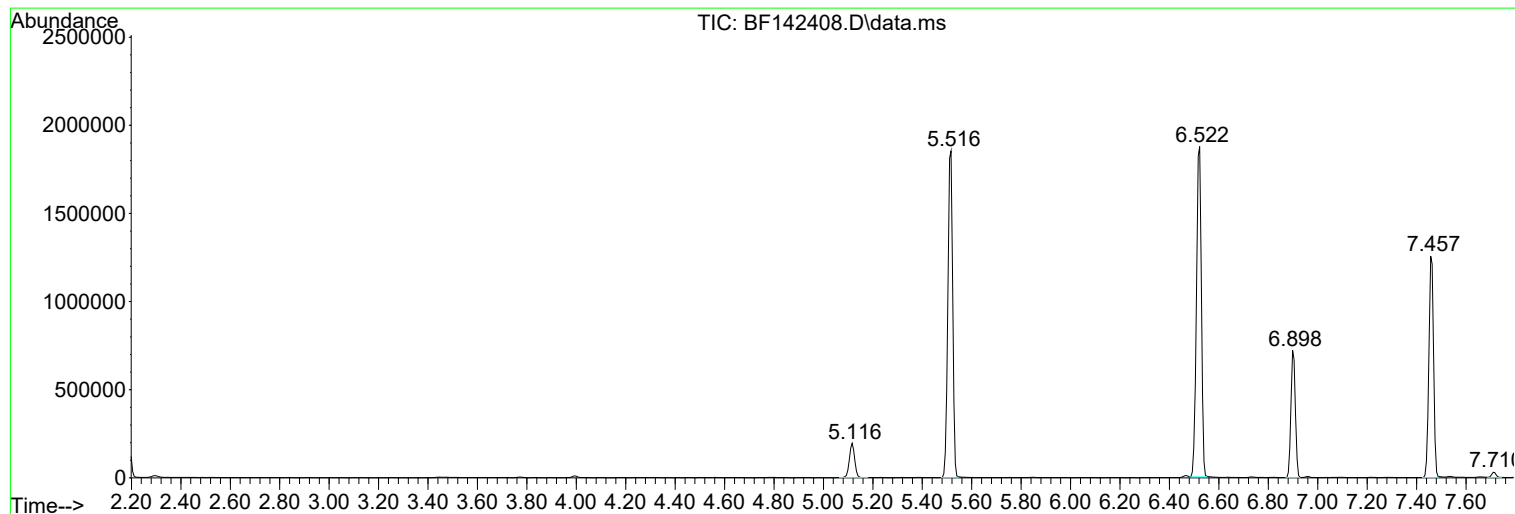
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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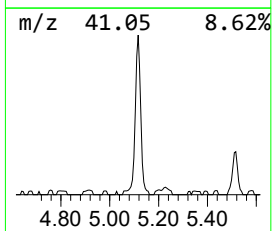
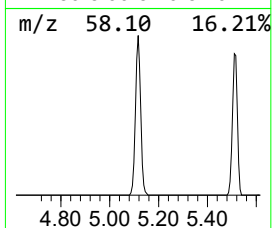
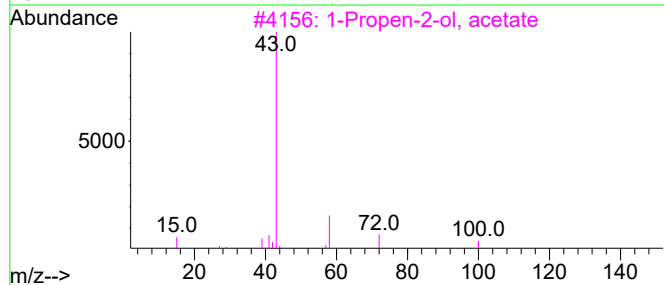
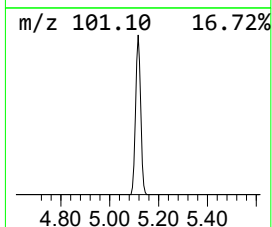
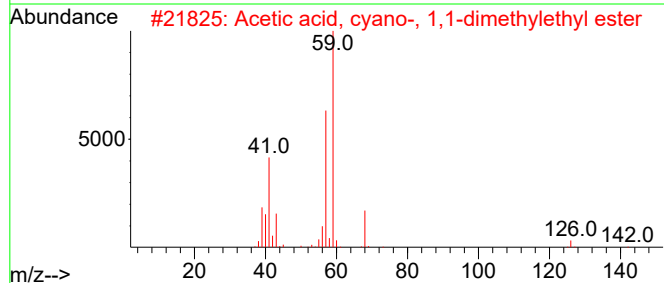
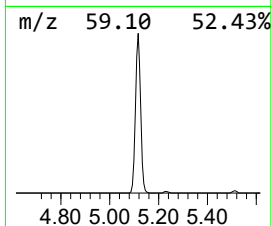
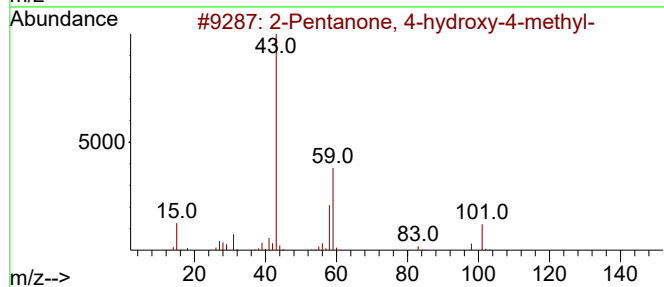
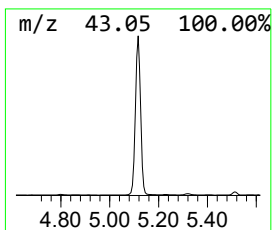
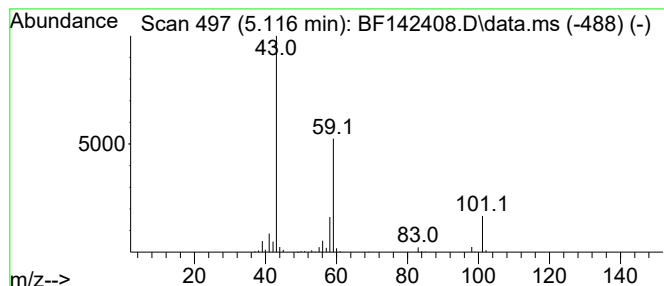
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	6.53 ng	290764	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9		
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9		



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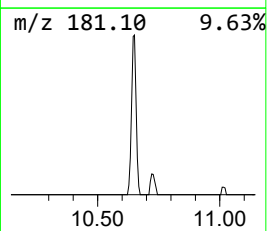
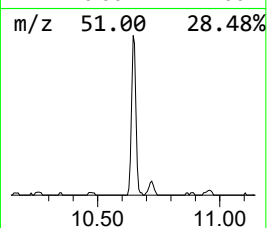
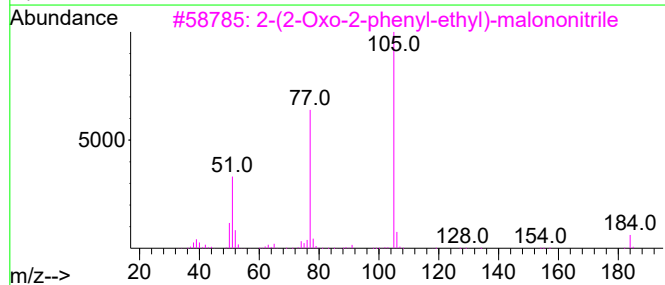
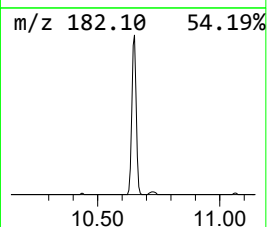
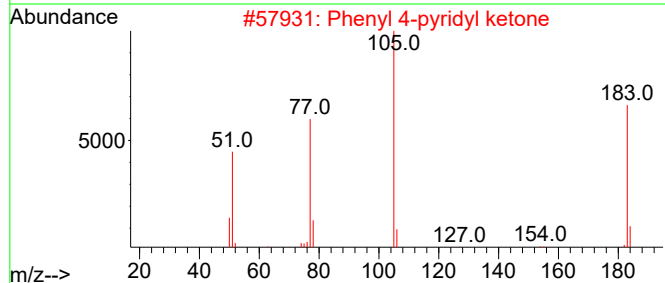
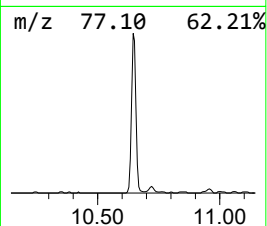
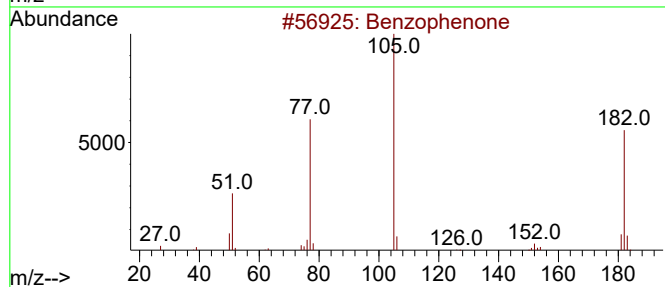
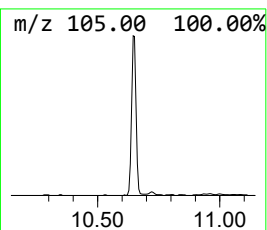
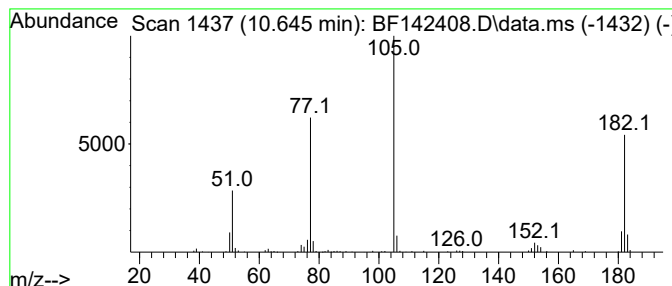
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.645	2.64 ng	172991	Acenaphthene-d10	9.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	53
4			Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47
5			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47



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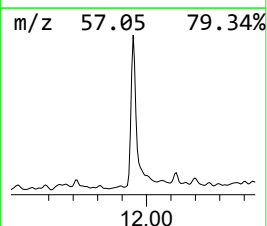
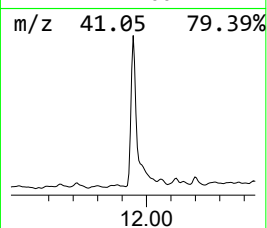
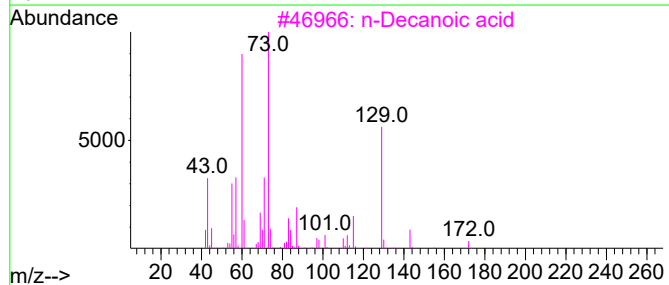
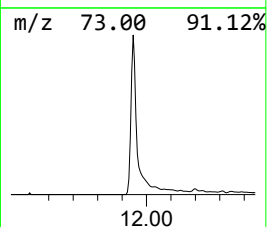
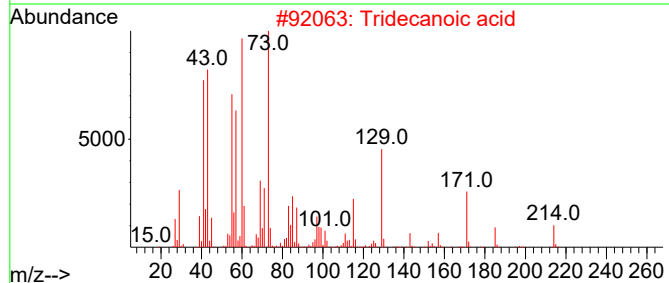
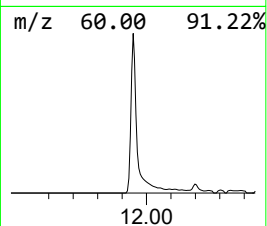
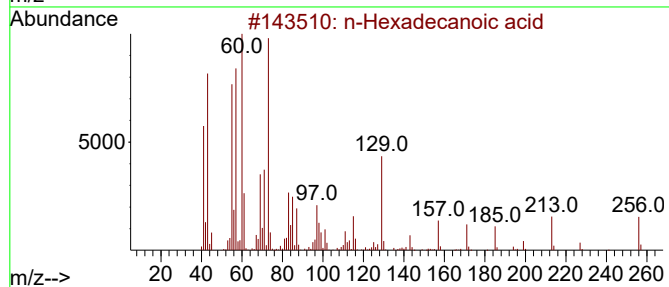
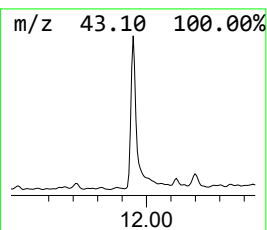
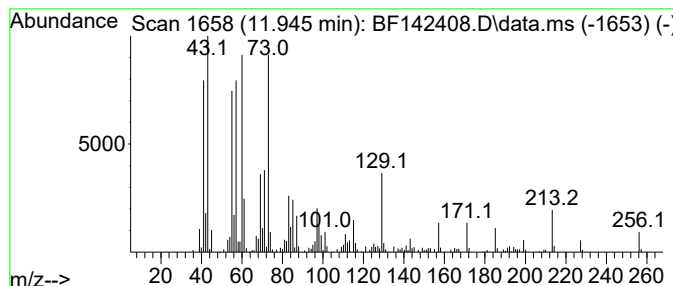
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	5.11 ng	302276	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			n-Decanoic acid	172	C10H20O2	000334-48-5	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Dodecanoic acid	200	C12H24O2	000143-07-7	70



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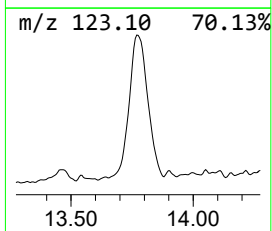
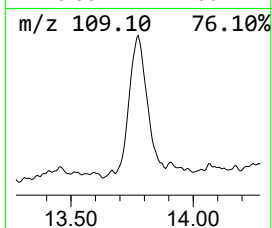
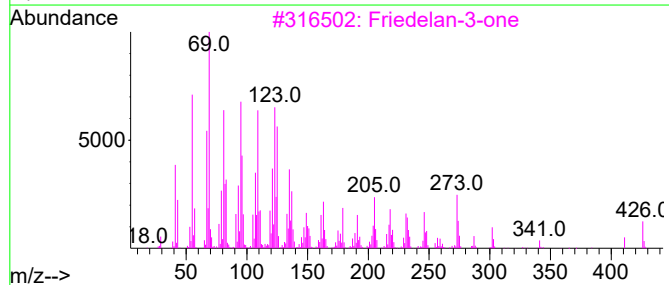
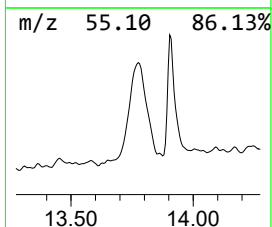
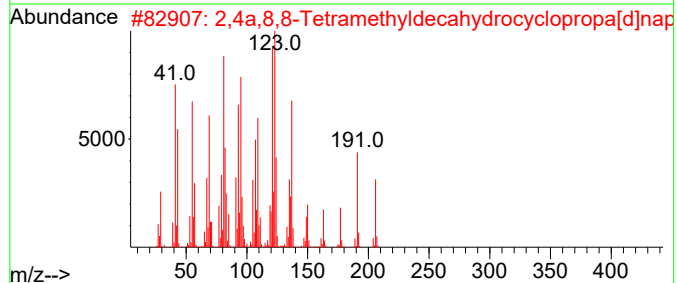
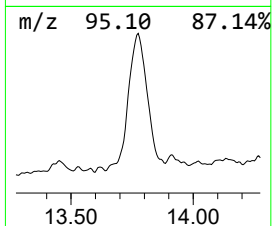
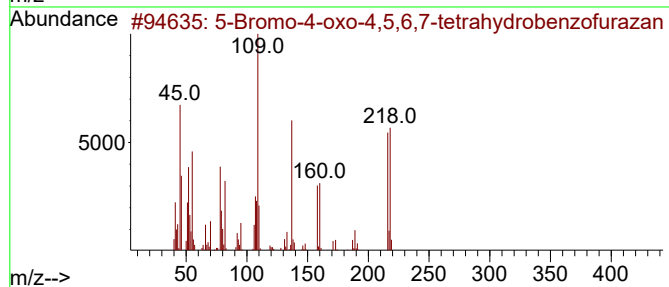
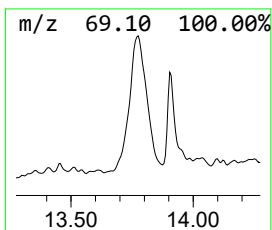
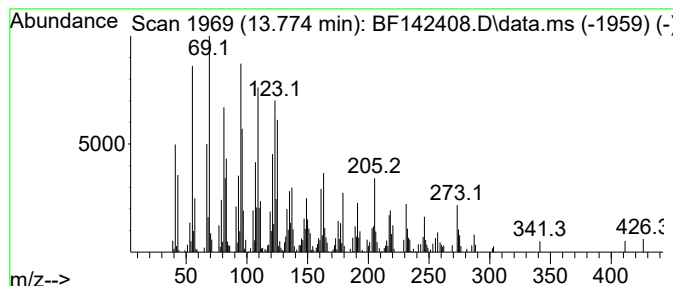
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Peak Number 4 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.774	13.19 ng	642137	Chrysene-d12		14.063	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	5-Bromo-4-oxo-4,5,6,7-tetrahydro...		216	C6H5BrN2O2	300574-36-1	68
2	2,4a,8,8-Tetramethyldecahydrocyc...		206	C15H26	074022-04-1	64
3	Friedelan-3-one		426	C30H50O	000559-74-0	62
4	(-)-Neoclovene-(II), dihydro-		206	C15H26	1000152-83-6	45
5	1,1,6-trimethyl-3-methylene-2-(3...		452	C33H56	1000373-94-5	41



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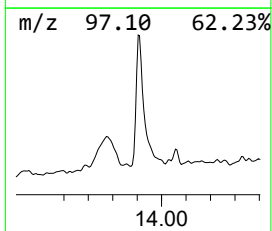
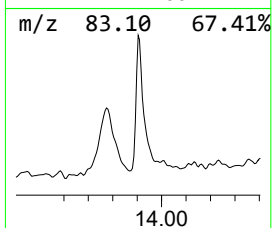
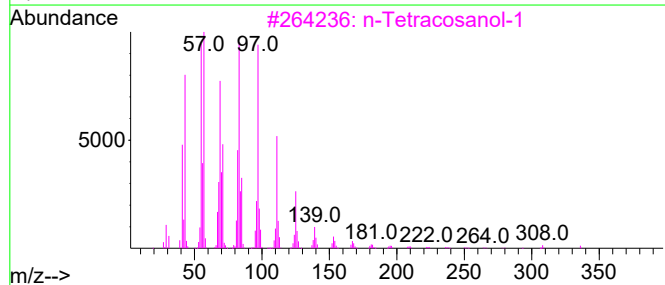
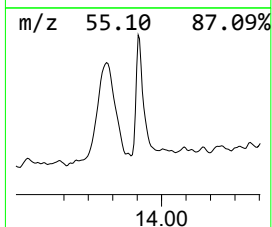
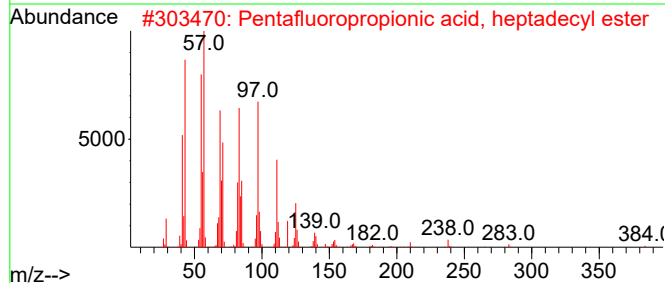
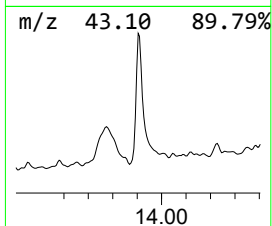
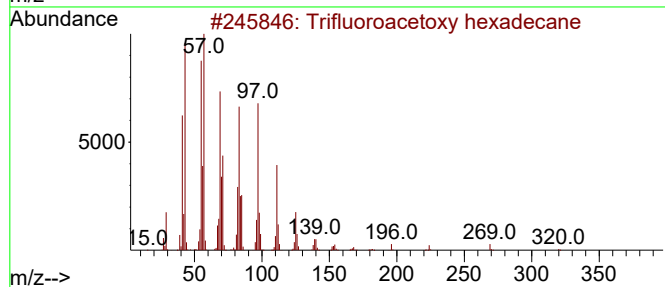
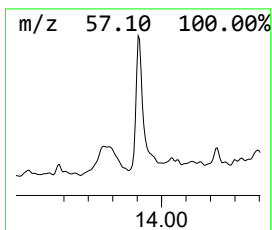
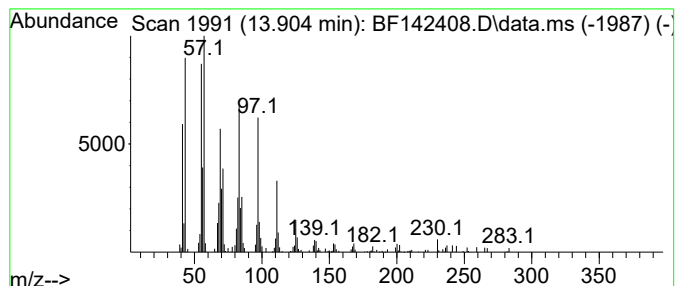
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Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.904	3.17 ng	154260	Chrysene-d12	14.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4	1-Octadecene	252	C18H36	000112-88-9	93
5	1-Heneicosanol	312	C21H44O	015594-90-8	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.116	6.5	ng	290764	1	6.898	890517	20.0
Benzophenone	10.645	2.6	ng	172991	3	9.939	1308650	20.0
n-Hexadecanoic ...	11.945	5.1	ng	302276	4	11.422	1182170	20.0
5-Bromo-4-oxo-4...	13.774	13.2	ng	642137	5	14.063	973350	20.0
Trifluoroacetox...	13.904	3.2	ng	154260	5	14.063	973350	20.0