

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090924\
 Data File : BF139284.D
 Acq On : 09 Sep 2024 15:48
 Operator : RC/JU
 Sample : P3888-02
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DN-W-02

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-BF090424.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139284.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.211	10	20	27	rVB	2214013	3506804	100.00%	14.684%
2	5.116	503	514	521	rVB	142455	243489	6.94%	1.020%
3	5.510	574	581	586	rBV	2178810	3050420	86.99%	12.773%
4	6.510	744	751	756	rBV	2233430	3178615	90.64%	13.310%
5	6.887	810	815	820	rBV	581812	699565	19.95%	2.929%
6	7.445	904	910	916	rBV	1484465	2037057	58.09%	8.530%
7	7.698	948	953	959	rVB	32823	39737	1.13%	0.166%
8	8.169	1027	1033	1038	rBV	695424	860450	24.54%	3.603%
9	9.245	1210	1216	1221	rBV	2562298	3257251	92.88%	13.640%
10	9.922	1326	1331	1336	rBV	700735	865468	24.68%	3.624%
11	10.639	1448	1453	1460	rBV	161501	204889	5.84%	0.858%
12	10.710	1460	1465	1479	rBV	1324419	1688189	48.14%	7.069%
13	11.410	1579	1584	1592	rBV	626974	781517	22.29%	3.273%
14	11.933	1666	1673	1685	rBV2	129249	205934	5.87%	0.862%
15	12.998	1848	1854	1859	rBV	1682209	2136395	60.92%	8.946%
16	13.904	2003	2008	2020	rBV	73807	147764	4.21%	0.619%
17	14.045	2027	2032	2043	rVB	410337	560159	15.97%	2.346%
18	15.521	2277	2283	2295	rBV	260005	417301	11.90%	1.747%

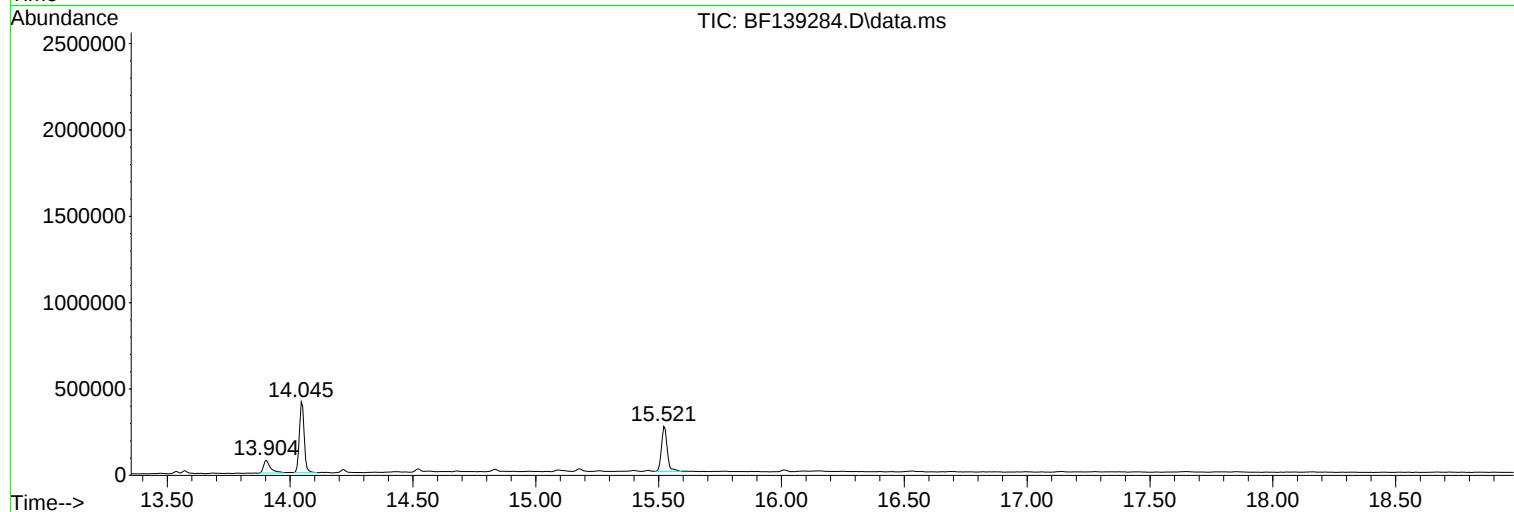
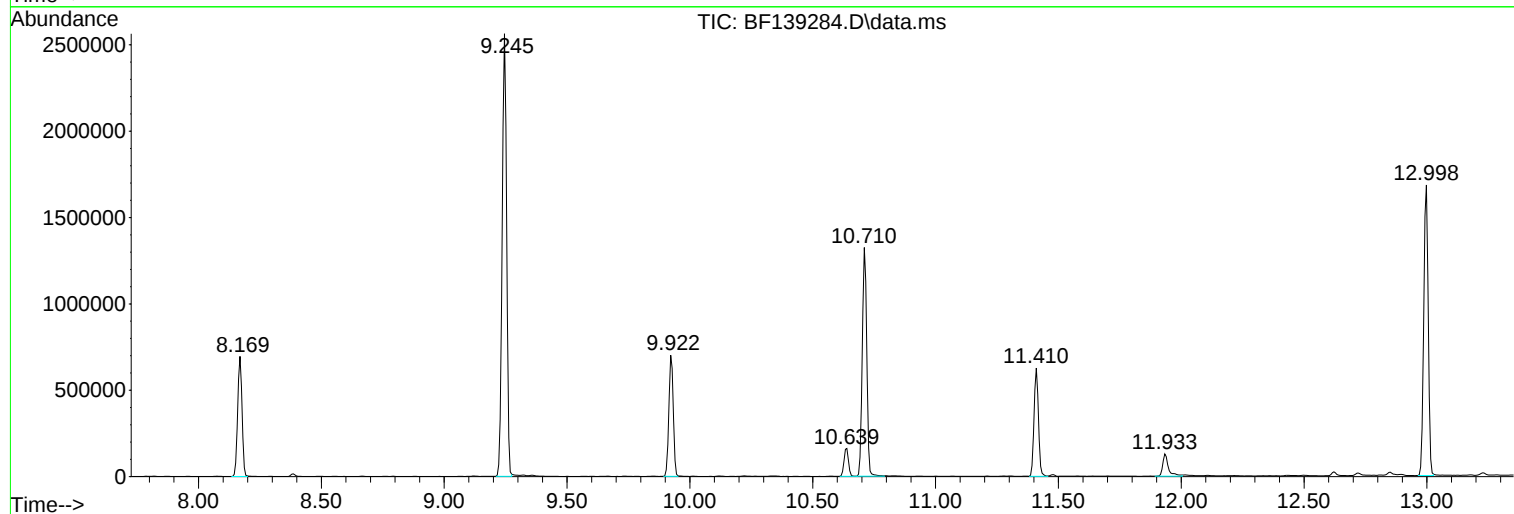
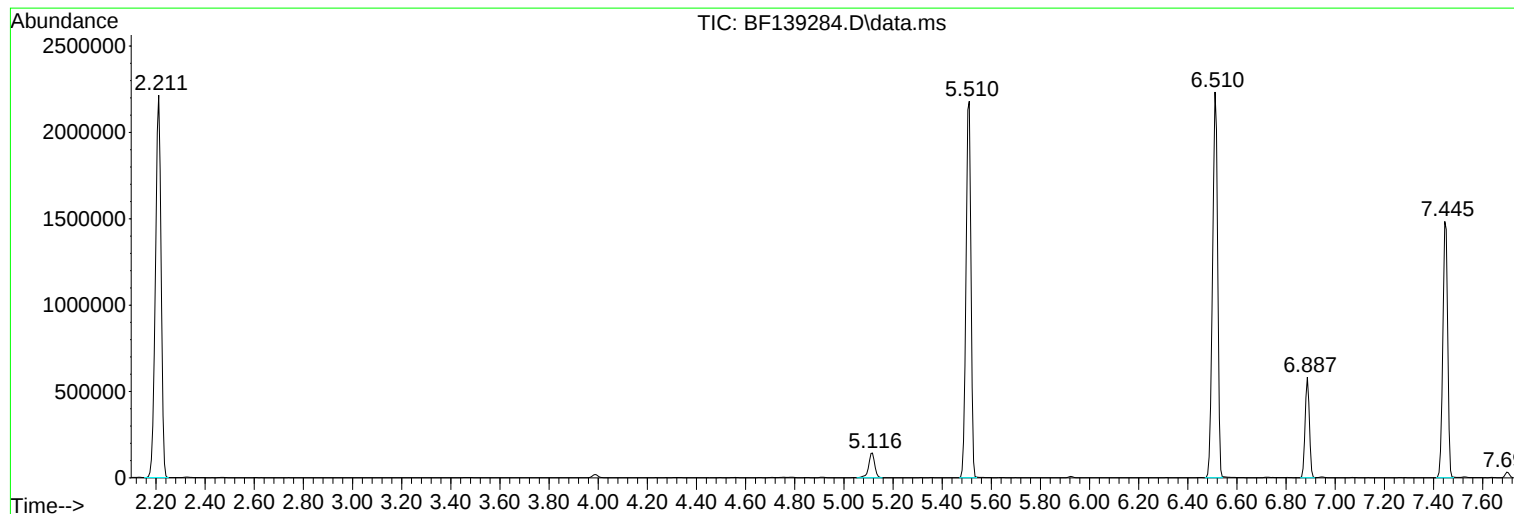
Sum of corrected areas: 23881004

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.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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Data File : BF139284.D
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Operator : RC/JU
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Instrument :
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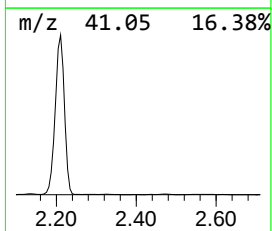
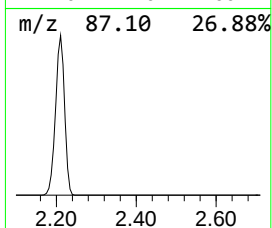
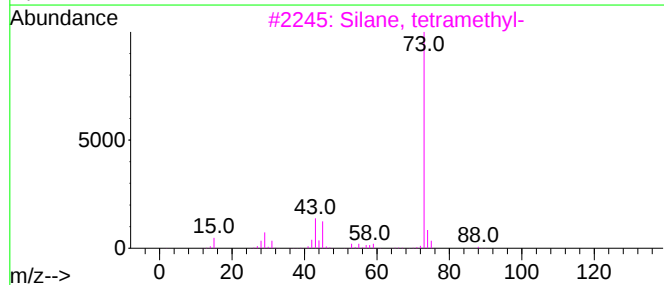
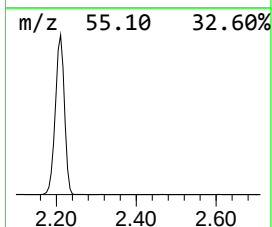
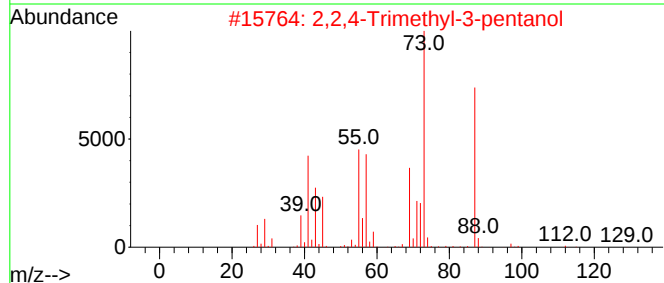
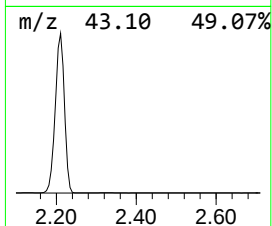
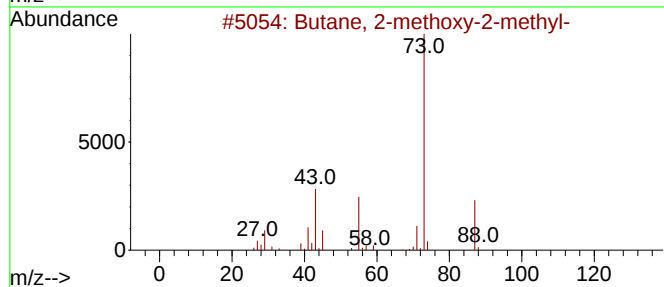
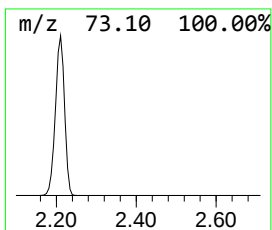
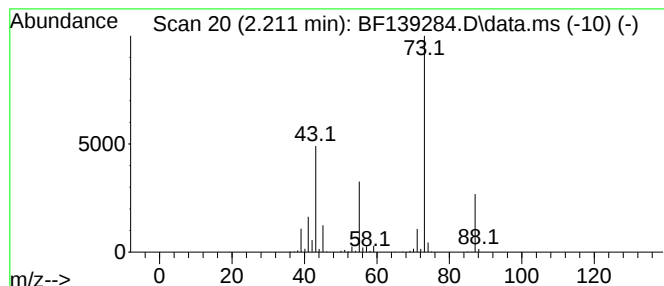
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.211	100.26 ng	3506800	1,4-Dichlorobenzene-d4	6.887

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	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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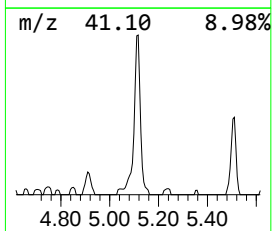
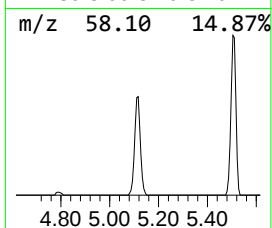
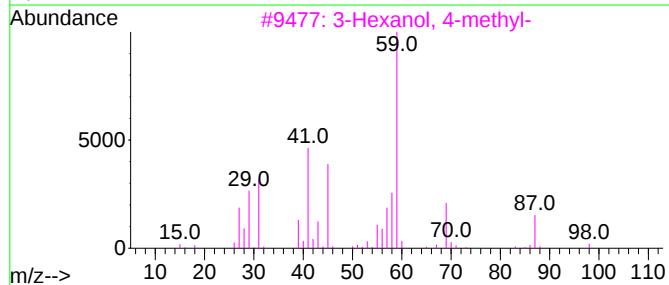
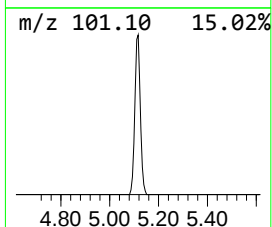
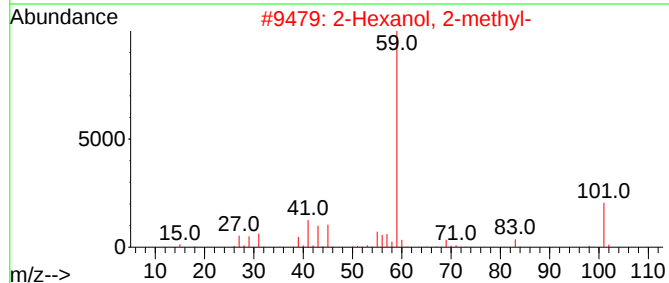
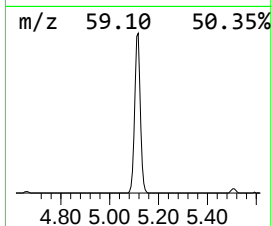
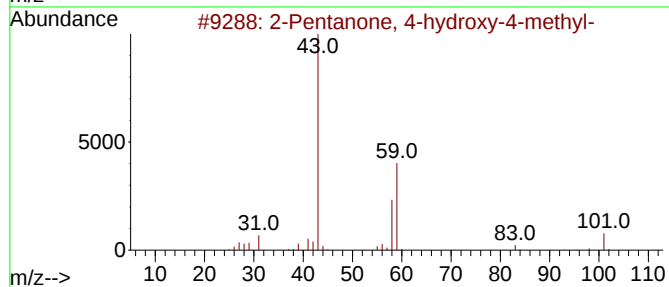
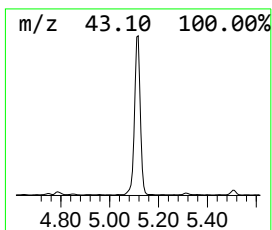
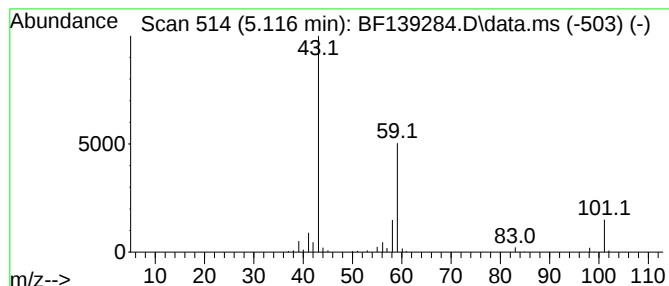
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	6.96 ng	243489	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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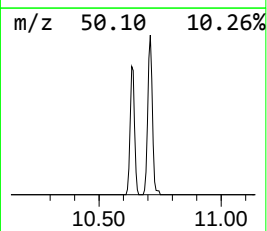
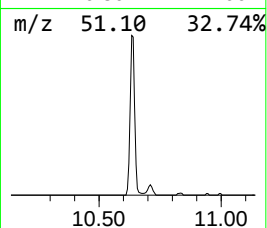
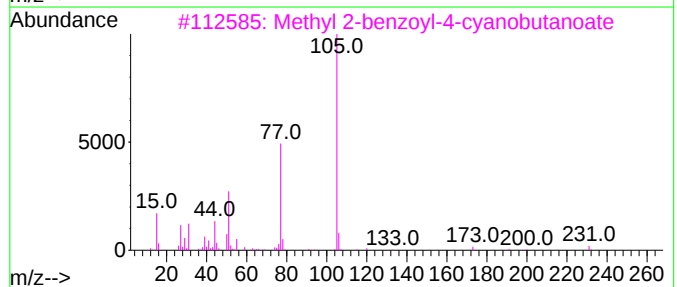
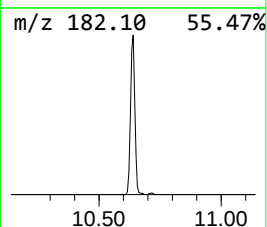
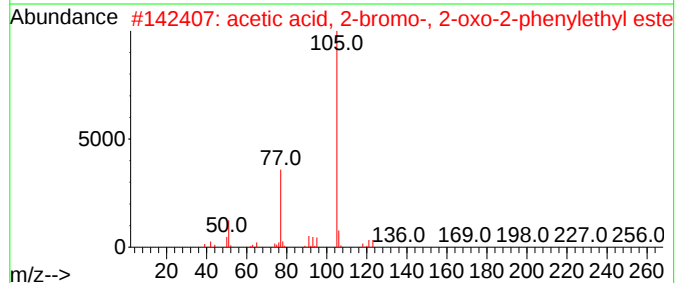
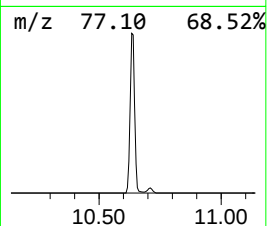
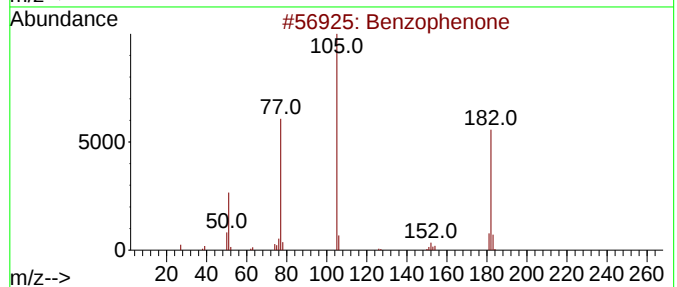
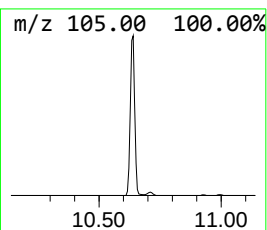
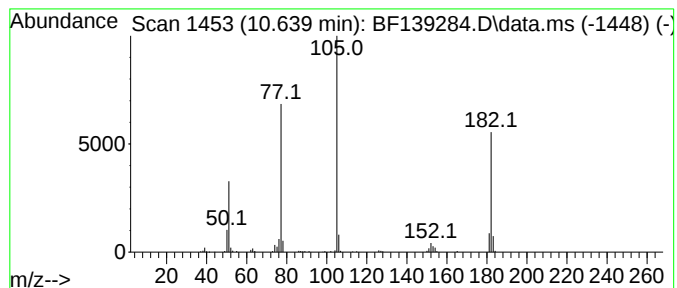
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.639	4.73 ng	204889	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	50
3			Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	50
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
5			N-cyanobenzamide	146	C8H6N2O	015150-25-1	50



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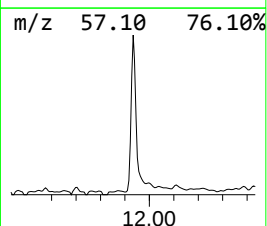
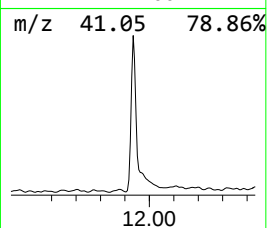
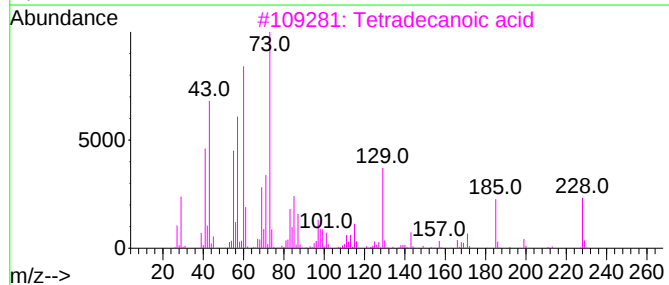
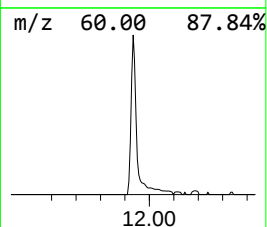
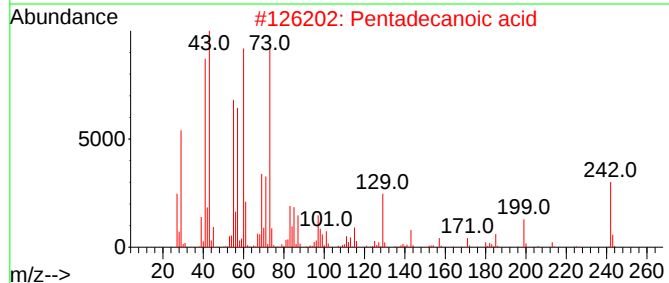
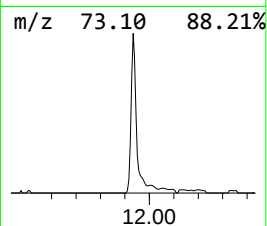
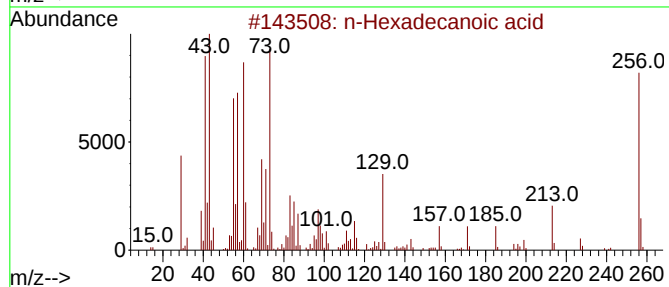
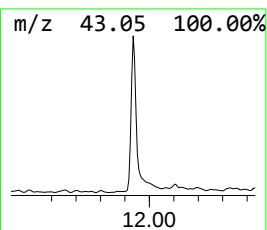
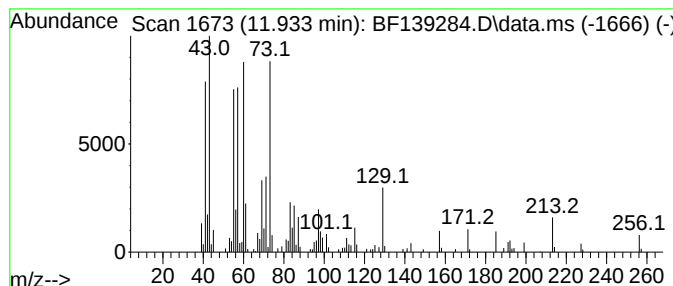
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	5.27 ng	205934	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Undecanoic acid	186	C11H22O2	000112-37-8	53



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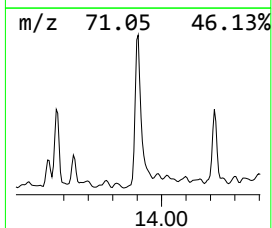
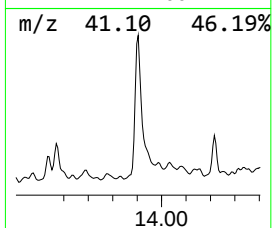
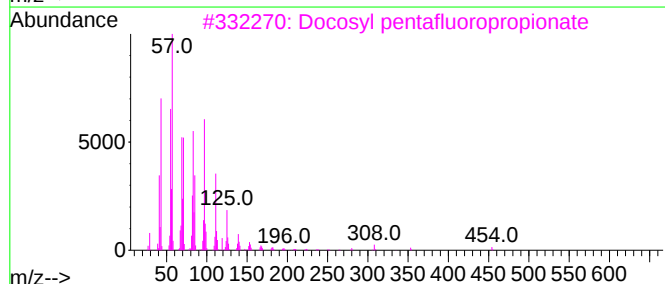
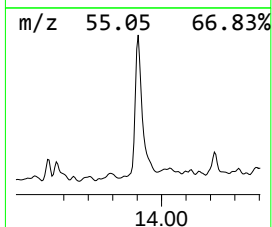
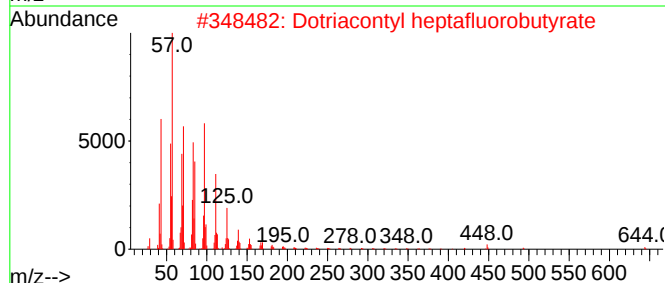
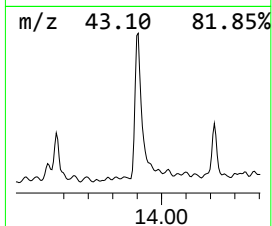
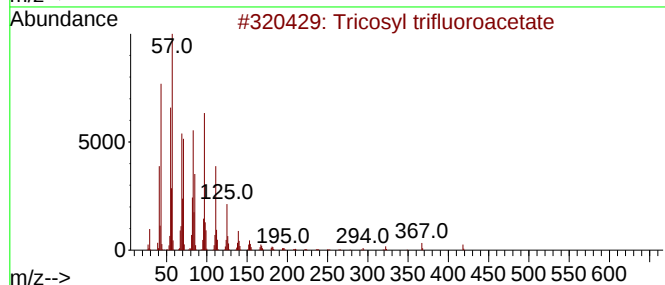
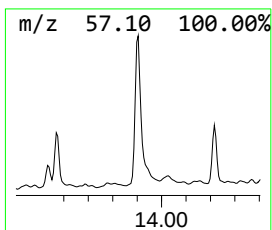
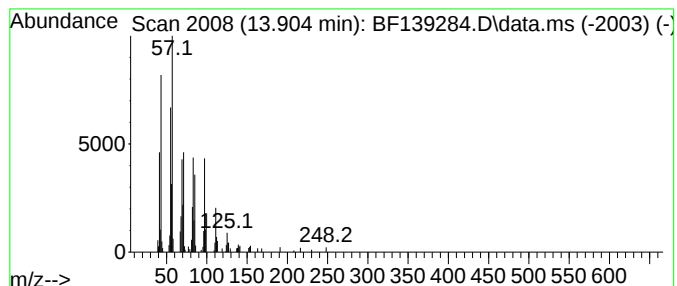
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Peak Number 5 Tricosyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	5.28 ng	147764	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
2			Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	91
3			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
4			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.211	100.3	ng	3506800	1	6.887	699565	20.0
2-Pentanone, 4-...	5.116	7.0	ng	243489	1	6.887	699565	20.0
Benzophenone	10.639	4.7	ng	204889	3	9.922	865468	20.0
n-Hexadecanoic ...	11.933	5.3	ng	205934	4	11.410	781517	20.0
Tricosyl triflu...	13.904	5.3	ng	147764	5	14.045	560159	20.0