

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110822\
 Data File : BF131060.D
 Acq On : 08 Nov 2022 11:30
 Operator : CG\JU
 Sample : N5415-16
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 R-29

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-BF110722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131060.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	10	24	29	rVB	172090	237486	10.34%	1.593%
2	2.340	38	43	48	rBV	18837	24404	1.06%	0.164%
3	4.516	408	413	420	rBV	37474	42554	1.85%	0.285%
4	5.134	513	518	531	rVB	399464	538797	23.46%	3.615%
5	5.528	579	585	588	rBV	2303127	2296597	100.00%	15.407%
6	6.528	749	755	758	rBV	1790791	1835810	79.94%	12.315%
7	6.898	814	818	821	rBV	456816	337560	14.70%	2.265%
8	7.463	909	914	917	rBV	1201946	1218943	53.08%	8.177%
9	8.181	1032	1036	1040	rBV	759227	702964	30.61%	4.716%
10	9.263	1214	1220	1223	rBV	2485610	2222534	96.78%	14.910%
11	9.945	1331	1336	1339	rBV	561075	493858	21.50%	3.313%
12	10.739	1466	1471	1474	rBV	1608392	1425646	62.08%	9.564%
13	11.439	1586	1590	1593	rBV	619410	507302	22.09%	3.403%
14	11.822	1651	1655	1658	rVB	46933	34383	1.50%	0.231%
15	12.227	1719	1724	1728	rBV3	23766	30697	1.34%	0.206%
16	13.033	1856	1861	1864	rBV	2204629	2139090	93.14%	14.350%
17	13.998	2016	2025	2034	rBV4	23618	81796	3.56%	0.549%
18	14.086	2036	2040	2044	rVB	457584	385605	16.79%	2.587%
19	14.939	2181	2185	2189	rVB	28087	27403	1.19%	0.184%
20	15.586	2289	2295	2302	rBV	260883	323110	14.07%	2.168%

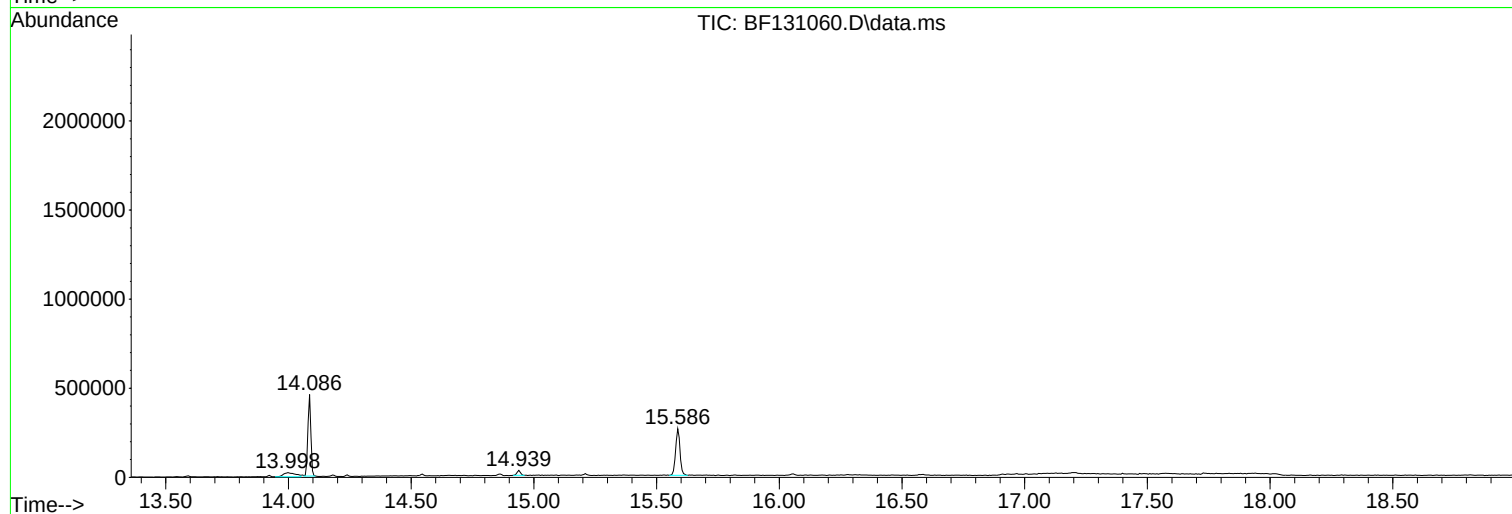
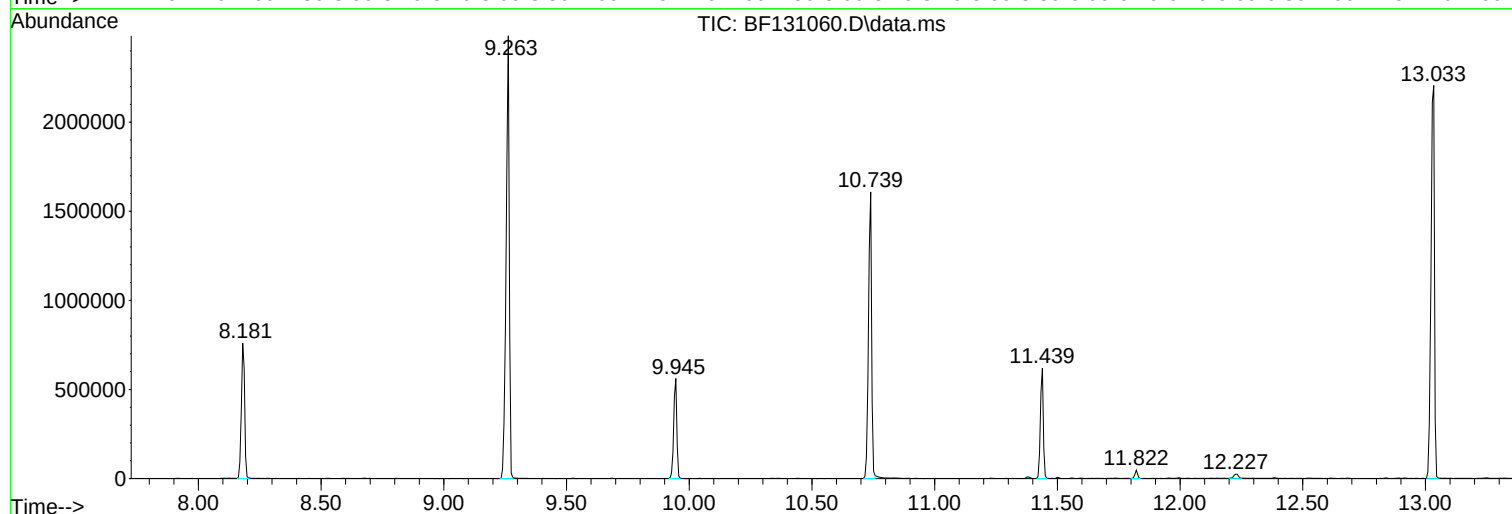
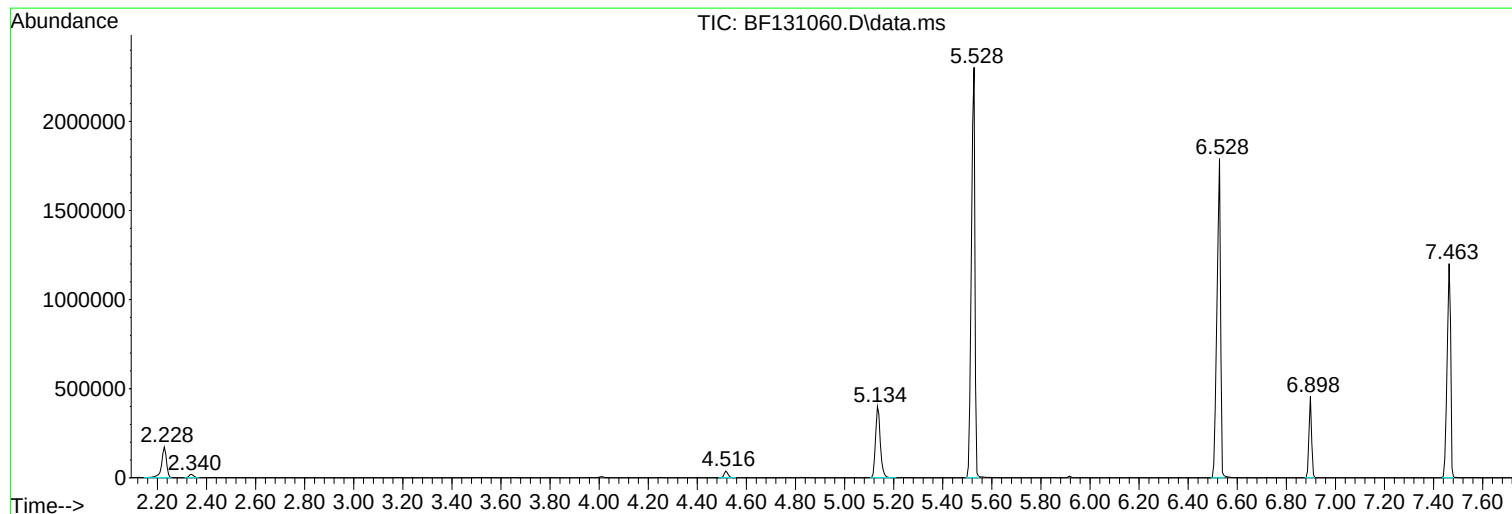
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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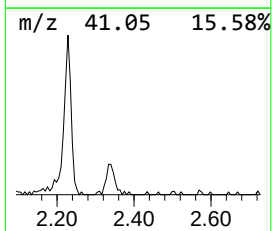
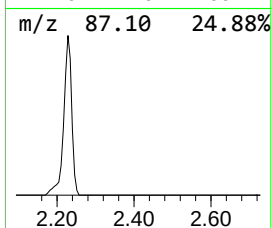
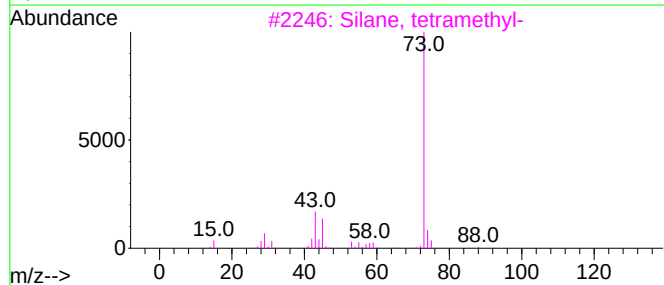
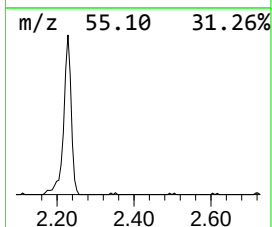
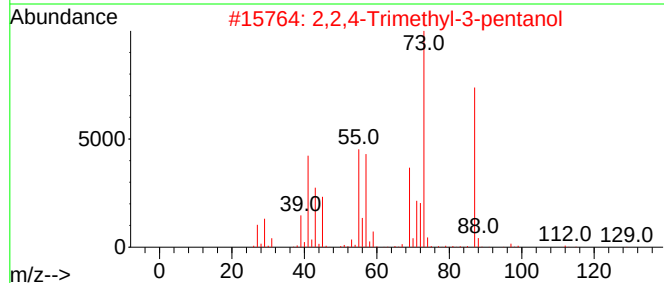
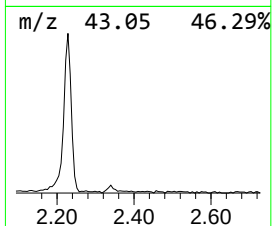
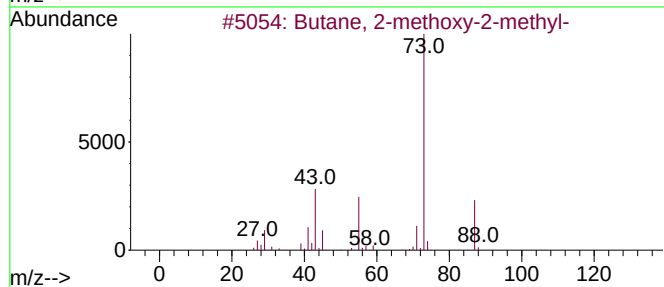
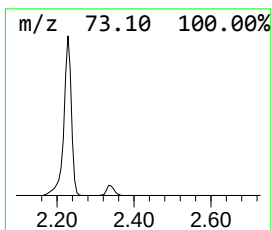
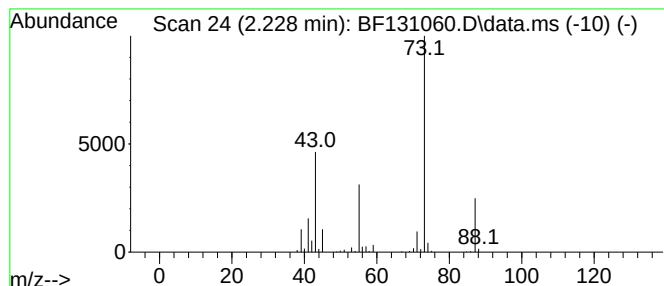
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	14.07 ng	237486	1,4-Dichlorobenzene-d4	6.898

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	17
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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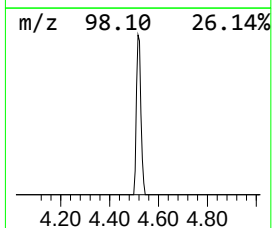
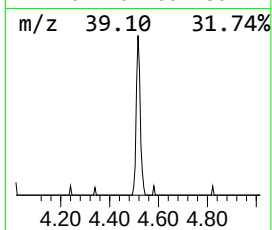
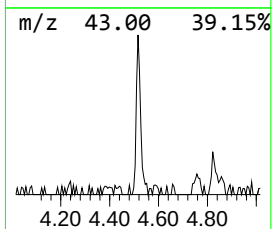
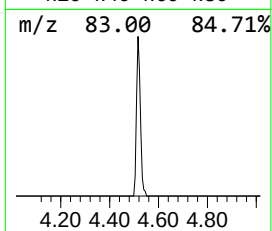
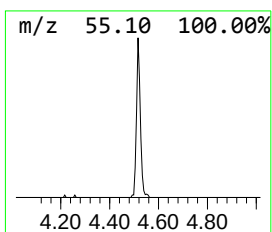
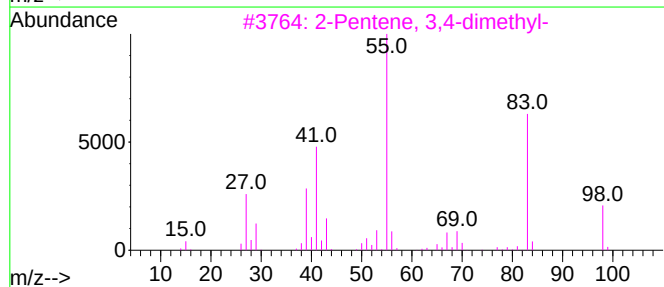
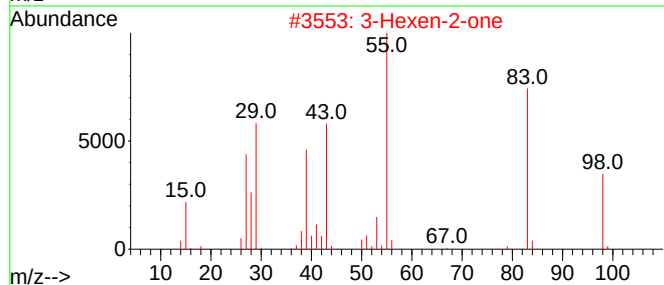
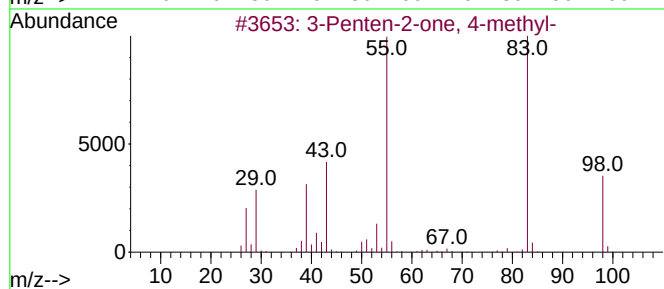
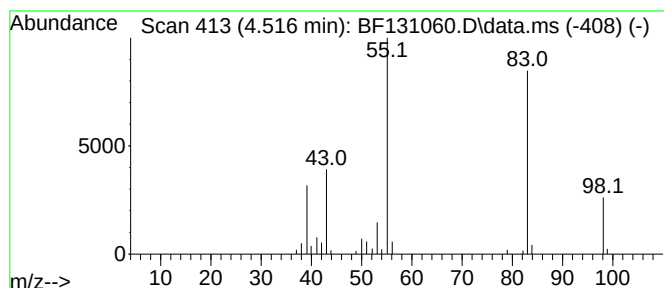
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.516	2.52 ng	42554	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	86
4			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80



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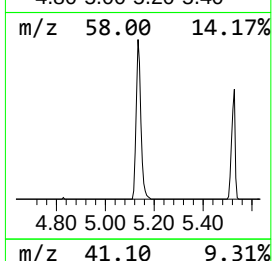
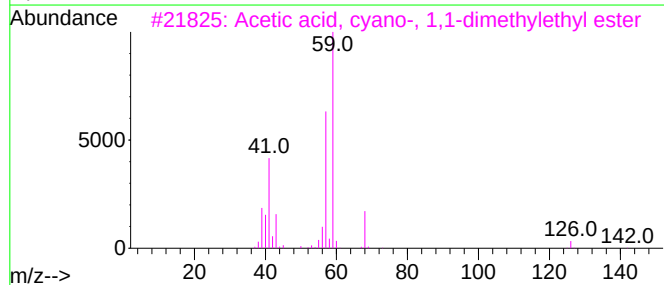
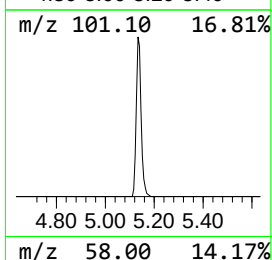
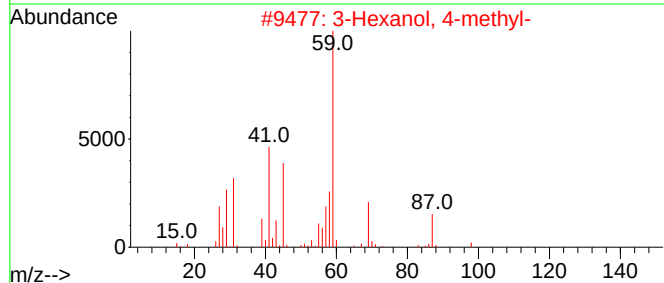
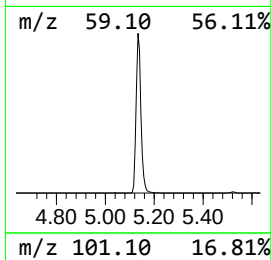
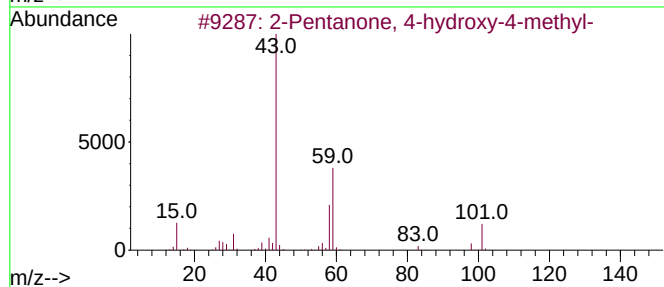
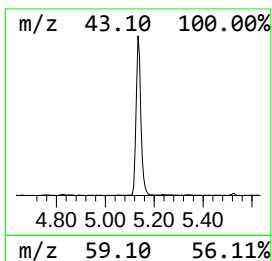
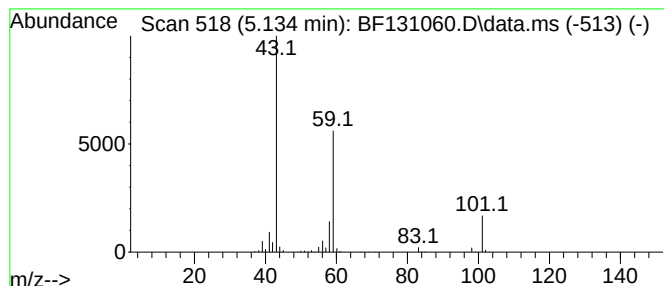
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.134	31.92 ng	538797	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	50
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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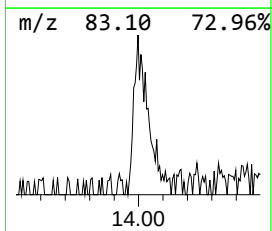
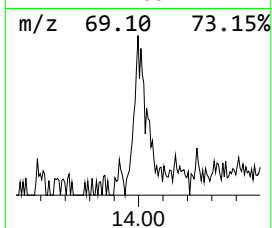
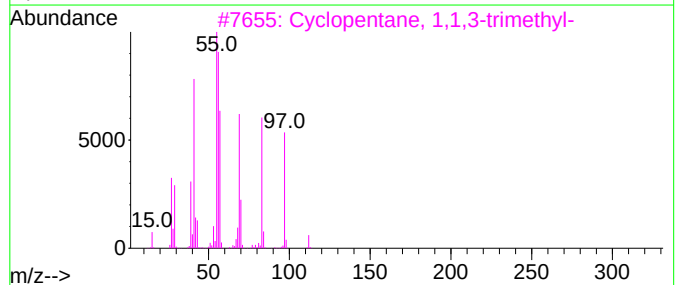
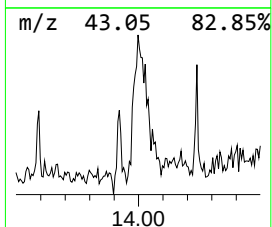
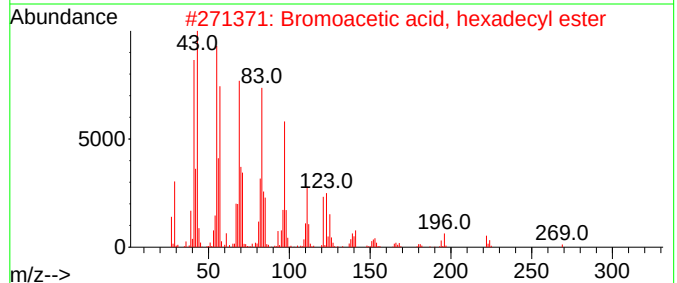
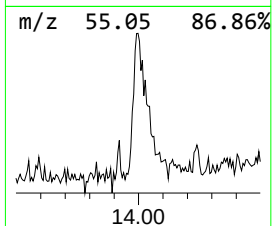
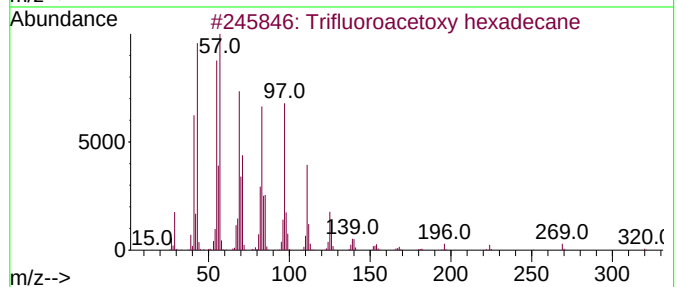
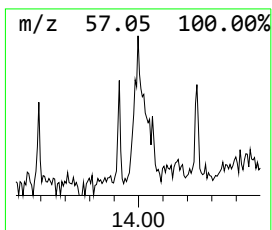
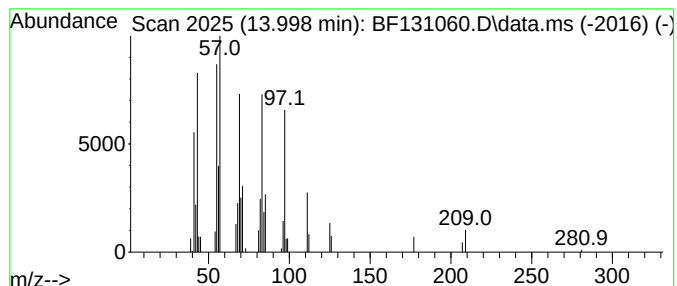
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Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	4.24 ng	81796	Chrysene-d12	14.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
2			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	74
3			Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	60
4			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	58
5			1-Octadecanol	270	C18H38O	000112-92-5	58



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.228	14.1	ng	237486	1	6.898	337560	20.0
3-Penten-2-one,...	4.516	2.5	ng	42554	1	6.898	337560	20.0
2-Pentanone, 4-...	5.134	31.9	ng	538797	1	6.898	337560	20.0
Trifluoroacetox...	13.998	4.2	ng	81796	5	14.086	385605	20.0