

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081224\
 Data File : BF138925.D
 Acq On : 12 Aug 2024 10:38
 Operator : RC/JU
 Sample : PB162487BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB162487BL

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-BF073024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138925.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	3	18	25	rVB	30688	57901	2.82%	0.479%
2	5.093	504	510	526	rBV	61848	112150	5.45%	0.928%
3	5.481	571	576	602	rBV	1261774	1722364	83.75%	14.257%
4	6.487	741	747	769	rBV	1253536	1753335	85.26%	14.514%
5	6.840	802	807	812	rBV	232284	281482	13.69%	2.330%
6	7.404	897	903	923	rBV	796547	1137786	55.33%	9.418%
7	8.122	1019	1025	1040	rBV	282016	374896	18.23%	3.103%
8	9.192	1201	1207	1212	rBV	1570469	2056512	100.00%	17.023%
9	9.875	1317	1323	1336	rVB	331556	432828	21.05%	3.583%
10	10.669	1452	1458	1478	rBV	853480	1163535	56.58%	9.632%
11	11.357	1570	1575	1591	rBV	334351	446287	21.70%	3.694%
12	12.751	1808	1812	1816	rVB	28663	33351	1.62%	0.276%
13	12.945	1839	1845	1850	rBV	1527931	1978951	96.23%	16.381%
14	13.457	1927	1932	1936	rBV	18213	23111	1.12%	0.191%
15	14.004	2019	2025	2036	rBV	184214	259696	12.63%	2.150%
16	15.039	2193	2201	2206	rBV3	9316	24452	1.19%	0.202%
17	15.468	2268	2274	2293	rVB	107003	198855	9.67%	1.646%
18	16.498	2440	2449	2465	rVB	5322	22985	1.12%	0.190%

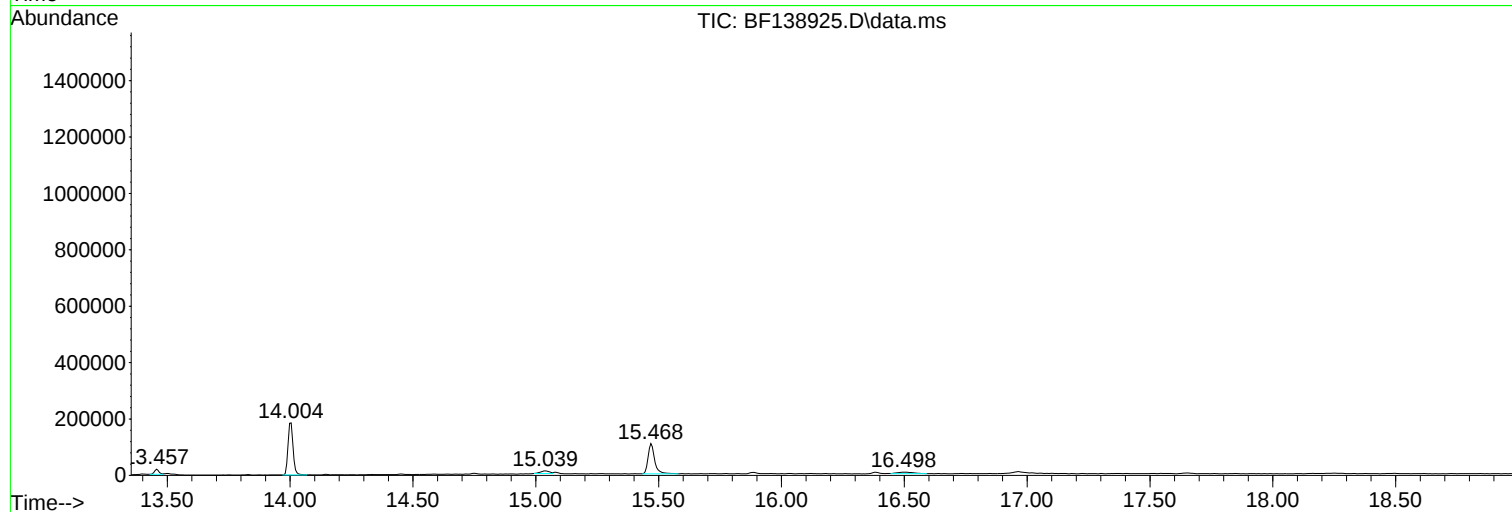
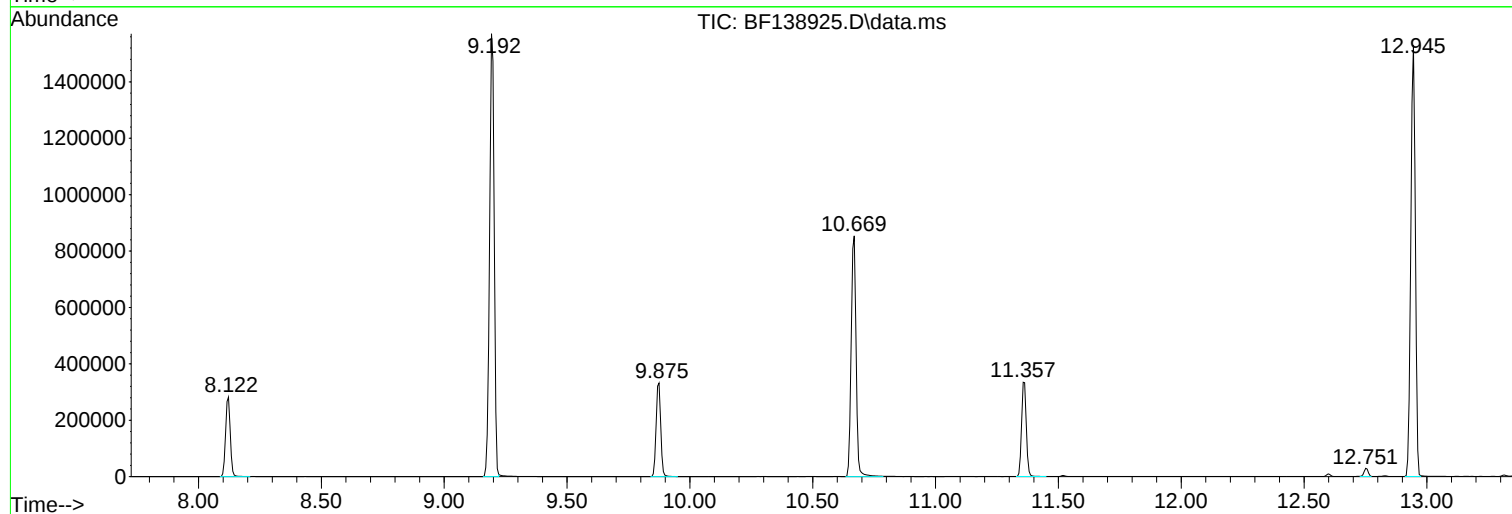
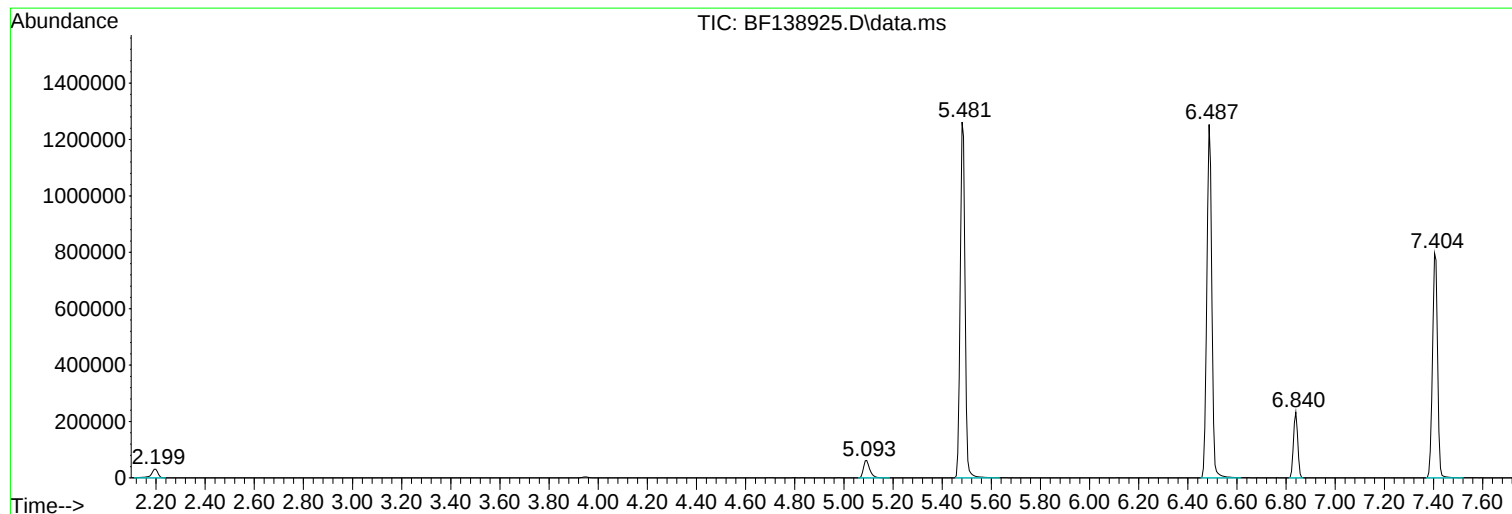
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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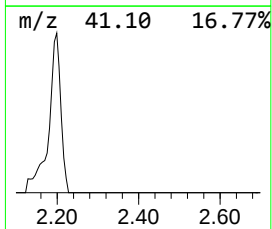
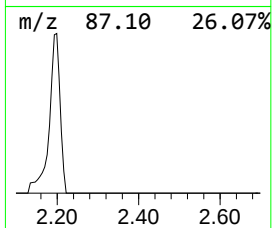
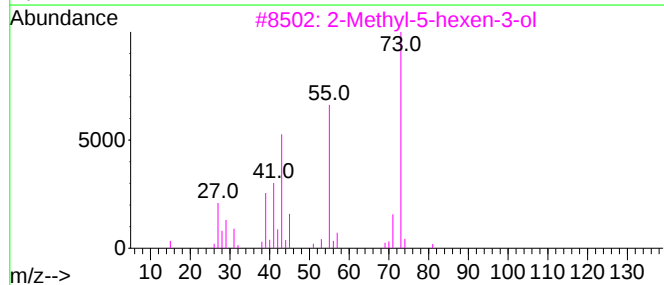
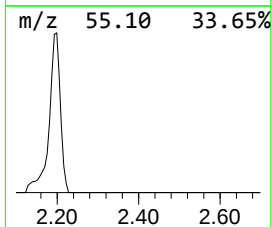
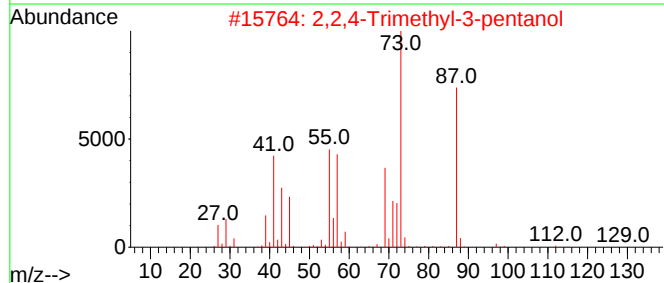
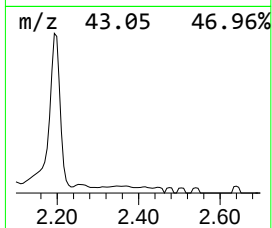
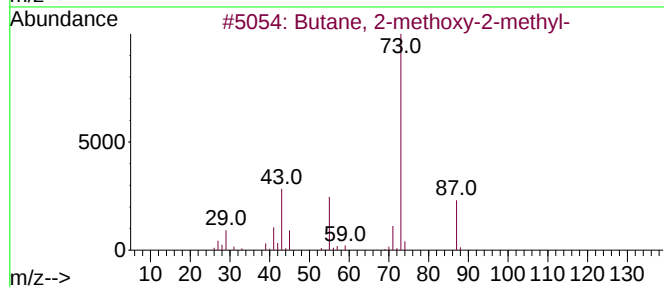
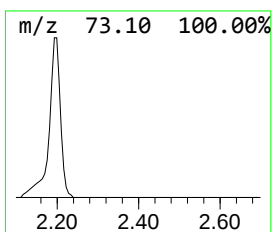
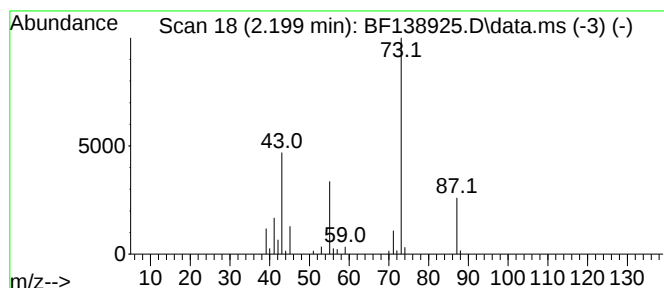
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.199	4.11 ng	57901	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	17



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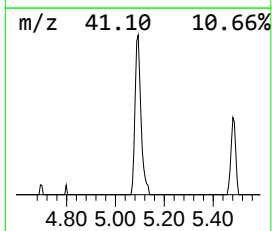
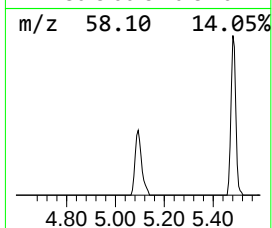
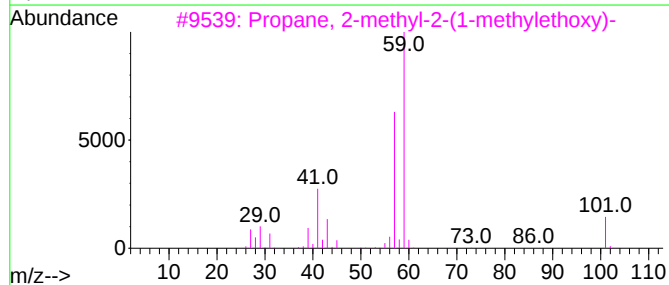
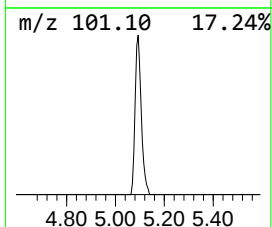
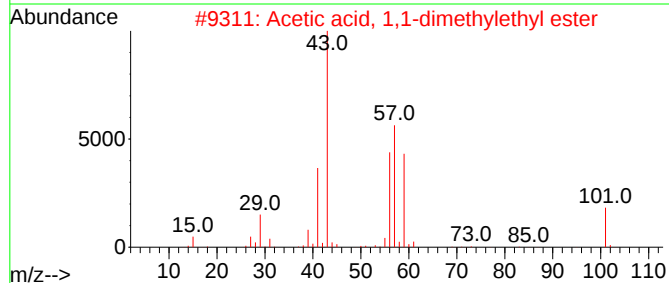
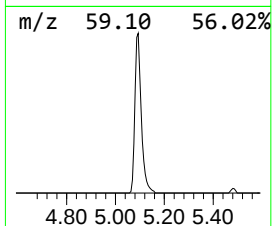
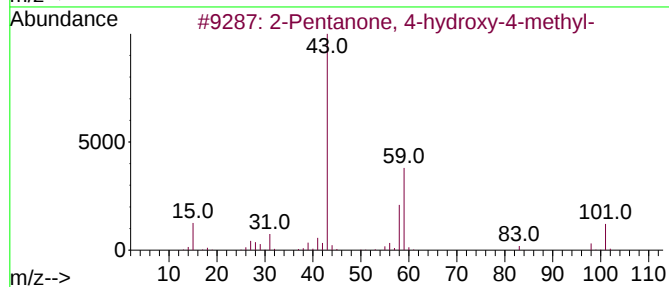
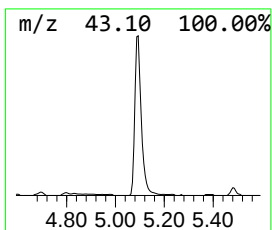
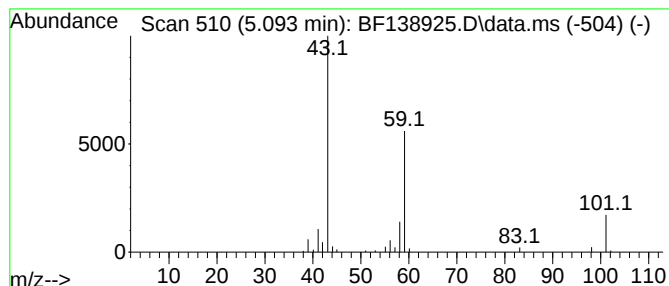
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.093	7.97 ng	112150	1,4-Dichlorobenzene-d4			6.840

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, 1,1-dimethylethyl e...	116	C6H12O2		000540-88-5	38
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O		017348-59-3	36
4	3-Hexanol, 4-methyl-	116	C7H16O		000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2		001116-98-9	25



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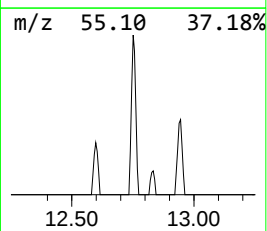
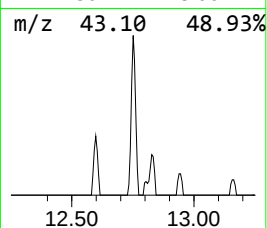
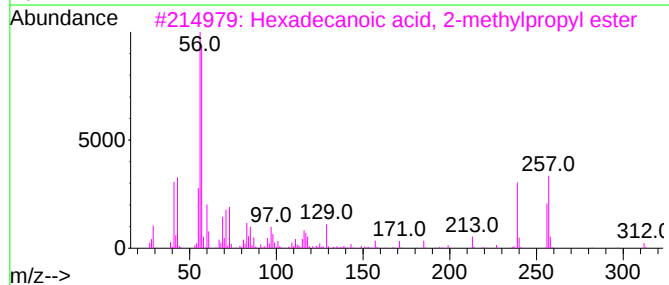
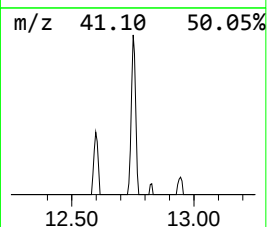
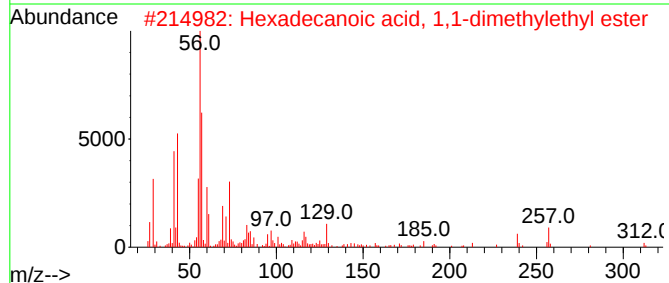
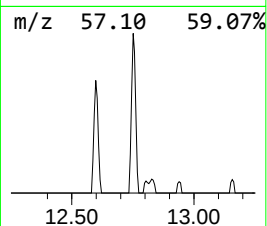
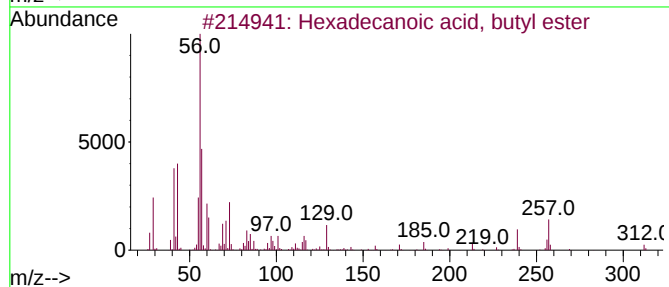
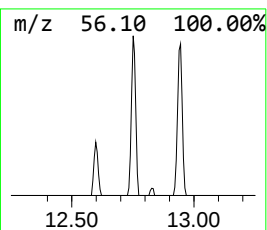
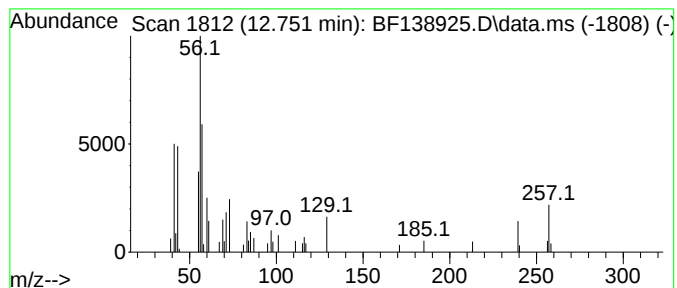
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.751	2.57 ng	33351	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	80
3			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	47
4			Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5			5-Methyl-2-hexanol, chlorodifluo...	228	C9H15ClF2O2	1010376-27-1	35



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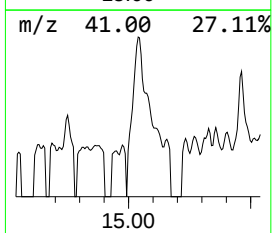
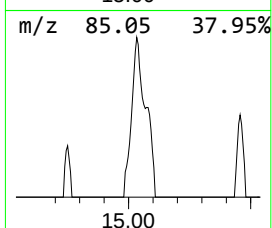
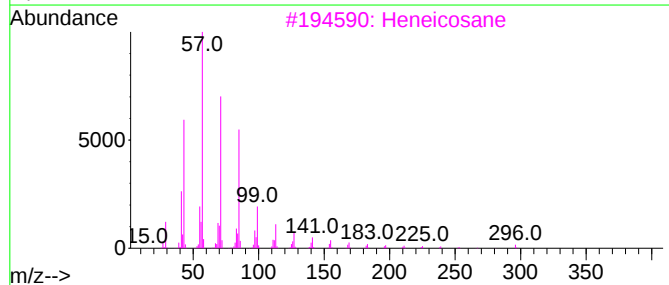
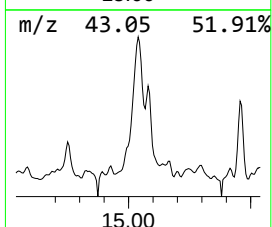
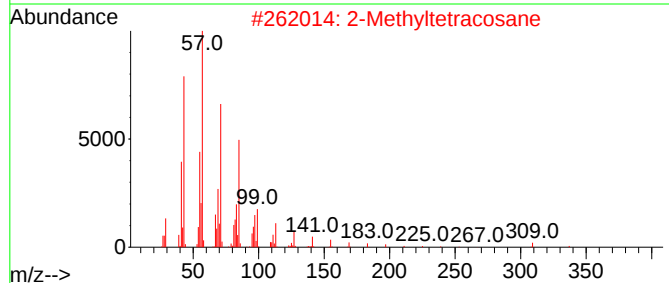
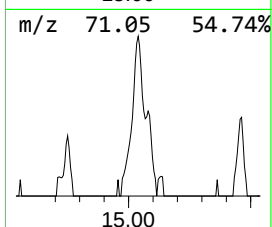
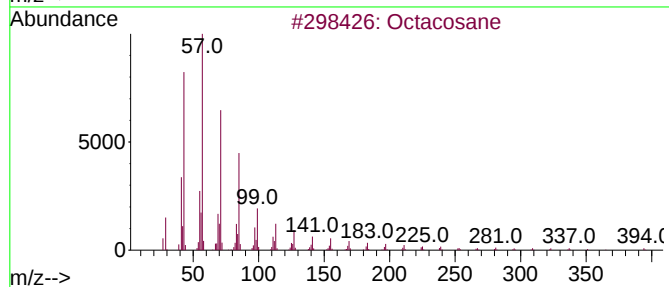
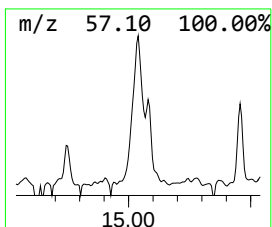
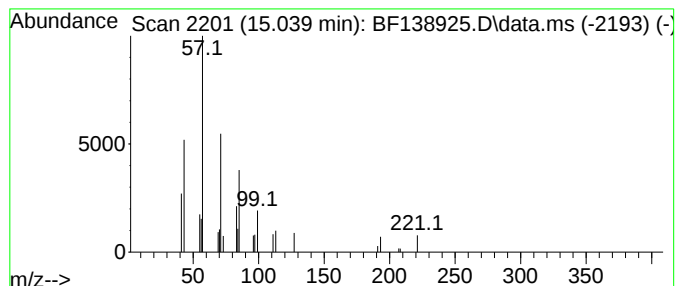
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Peak Number 4 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.039	2.46 ng	24452	Perylene-d12	15.469

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	80
2		2-Methyltetracosane	352	C25H52	001560-78-7	72
3		Heneicosane	296	C21H44	000629-94-7	59
4		Pentadecane	212	C15H32	000629-62-9	59
5		Hentriacontane	437	C31H64	000630-04-6	53



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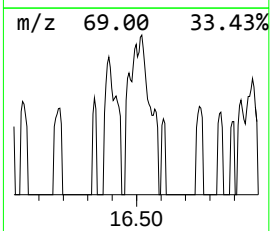
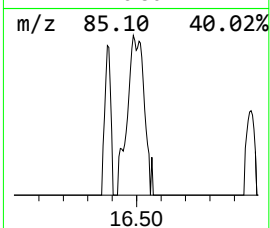
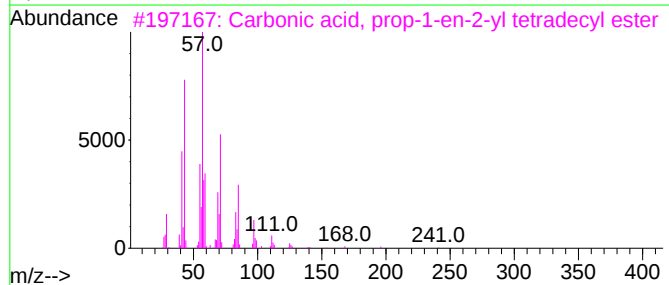
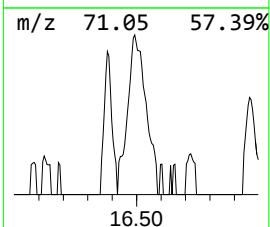
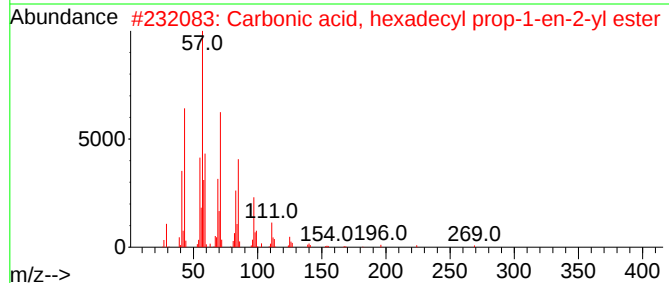
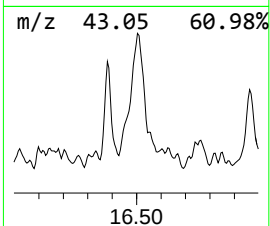
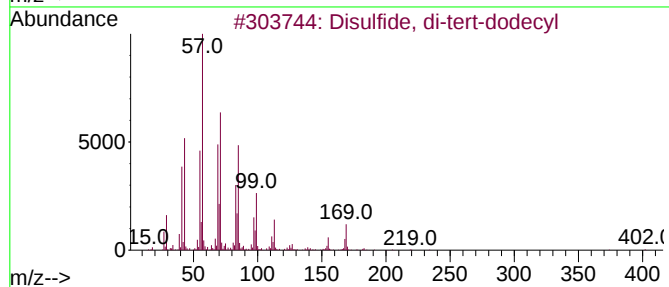
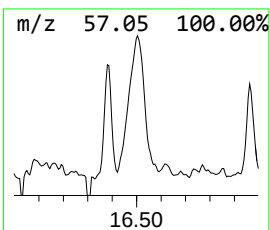
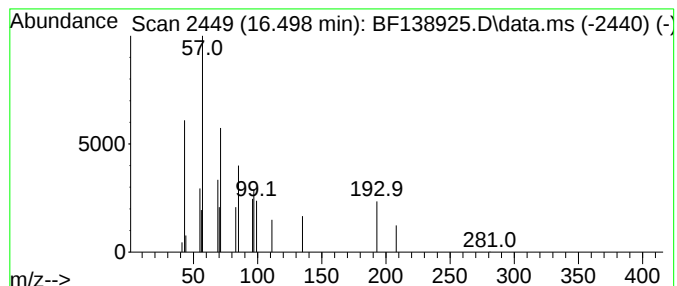
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Disulfide, di-tert-dodecyl Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.498	2.31 ng	22985	Perylene-d12	15.469

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	50
2			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	50
3			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	50
4			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	47
5			Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	47



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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...	2.199	4.1	ng	57901	1	6.840	281482	20.0
2-Pentanone, 4-...	5.093	8.0	ng	112150	1	6.840	281482	20.0
Hexadecanoic ac...	12.751	2.6	ng	33351	5	14.004	259696	20.0
Octacosane	15.039	2.5	ng	24452	6	15.469	198855	20.0
Disulfide, di-t...	16.498	2.3	ng	22985	6	15.469	198855	20.0