

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111522\
 Data File : BF131244.D
 Acq On : 15 Nov 2022 21:44
 Operator : CG\JU
 Sample : PB148901BL
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB148901BL

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-BF111522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131244.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.346	34	44	49	rBV	111761	149161	3.77%	0.588%
2	5.210	525	531	542	rBV	611784	851772	21.53%	3.356%
3	5.593	590	596	599	rBV	2875774	3123062	78.94%	12.305%
4	5.987	660	663	666	rBV	54560	43299	1.09%	0.171%
5	6.587	759	765	768	rBV	2546459	3177024	80.30%	12.518%
6	6.975	827	831	834	rVB	830044	682772	17.26%	2.690%
7	7.540	921	927	930	rBV	1869956	1974640	49.91%	7.780%
8	8.263	1045	1050	1053	rBV	1062614	929476	23.49%	3.662%
9	9.345	1228	1234	1237	rBV	3652724	3656971	92.44%	14.409%
10	10.028	1345	1350	1354	rBV	1266754	1096803	27.72%	4.321%
11	10.822	1478	1485	1488	rBV	2555110	2385478	60.30%	9.399%
12	11.528	1601	1605	1608	rVB	1348074	1127049	28.49%	4.441%
13	13.127	1872	1877	1880	rBV	4203356	3956253	100.00%	15.588%
14	14.180	2052	2056	2060	rBV	1157030	1026320	25.94%	4.044%
15	15.363	2252	2257	2265	rVB	46150	57554	1.45%	0.227%
16	15.727	2313	2319	2324	rBV	649580	803996	20.32%	3.168%
17	15.780	2324	2328	2334	rVB2	59660	83822	2.12%	0.330%
18	16.262	2404	2410	2419	rBV2	45577	80432	2.03%	0.317%
19	16.827	2499	2506	2517	rBV2	33946	75054	1.90%	0.296%
20	17.492	2609	2619	2627	rBV5	20149	53579	1.35%	0.211%
21	18.274	2744	2752	2761	rBV6	16194	46117	1.17%	0.182%

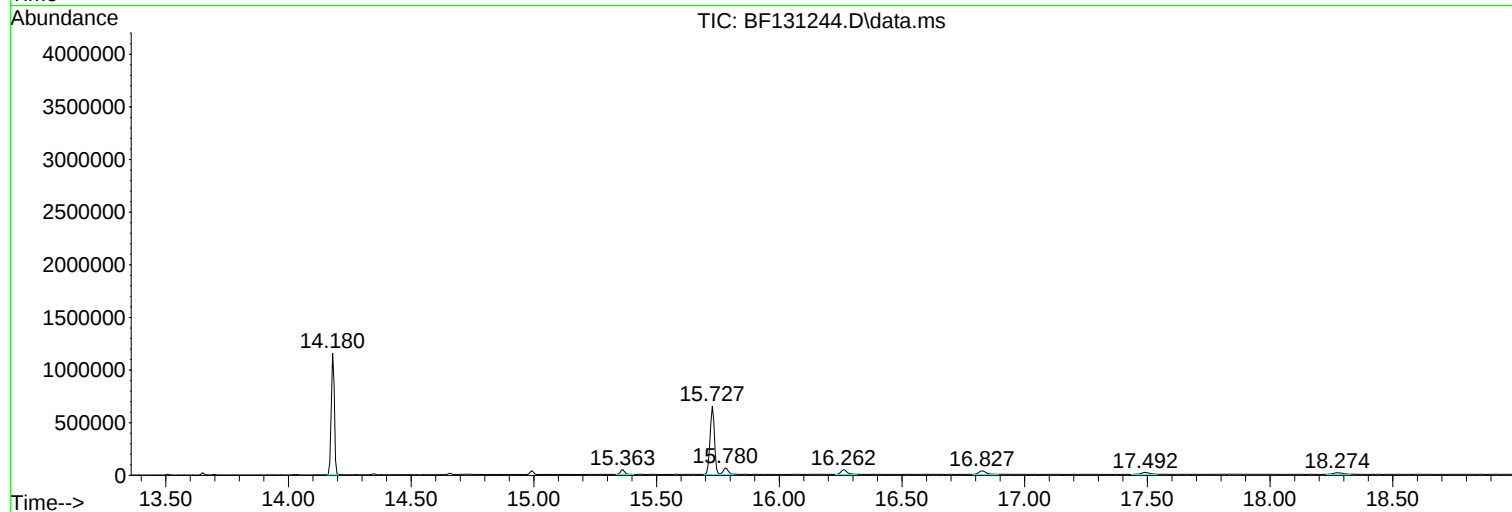
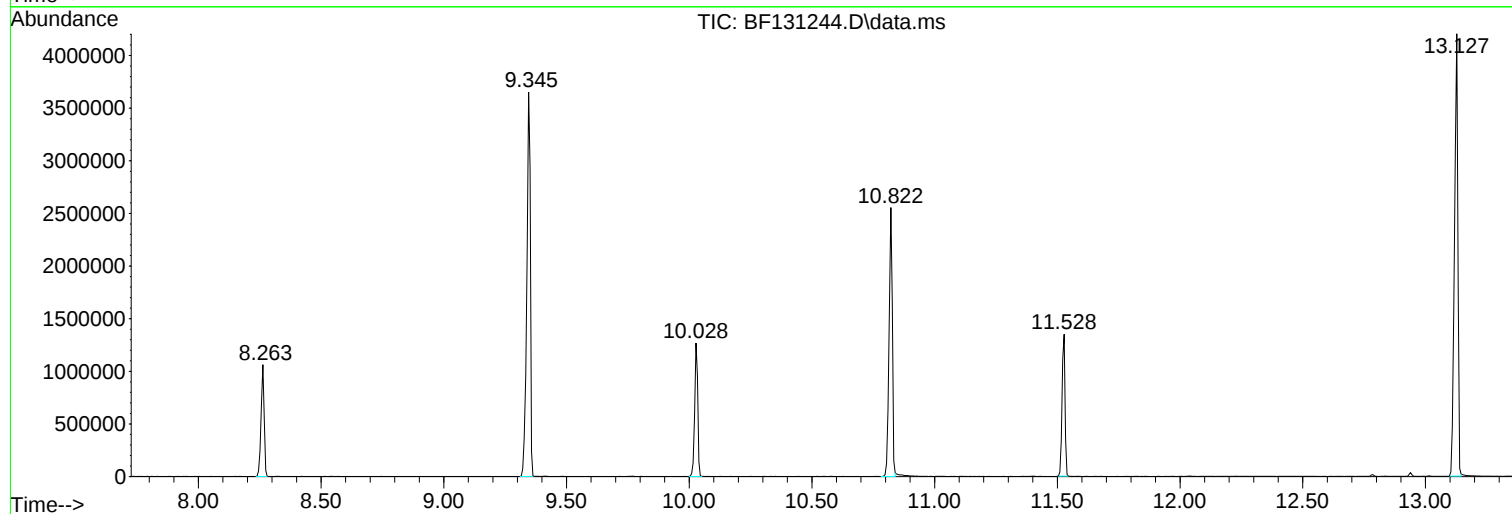
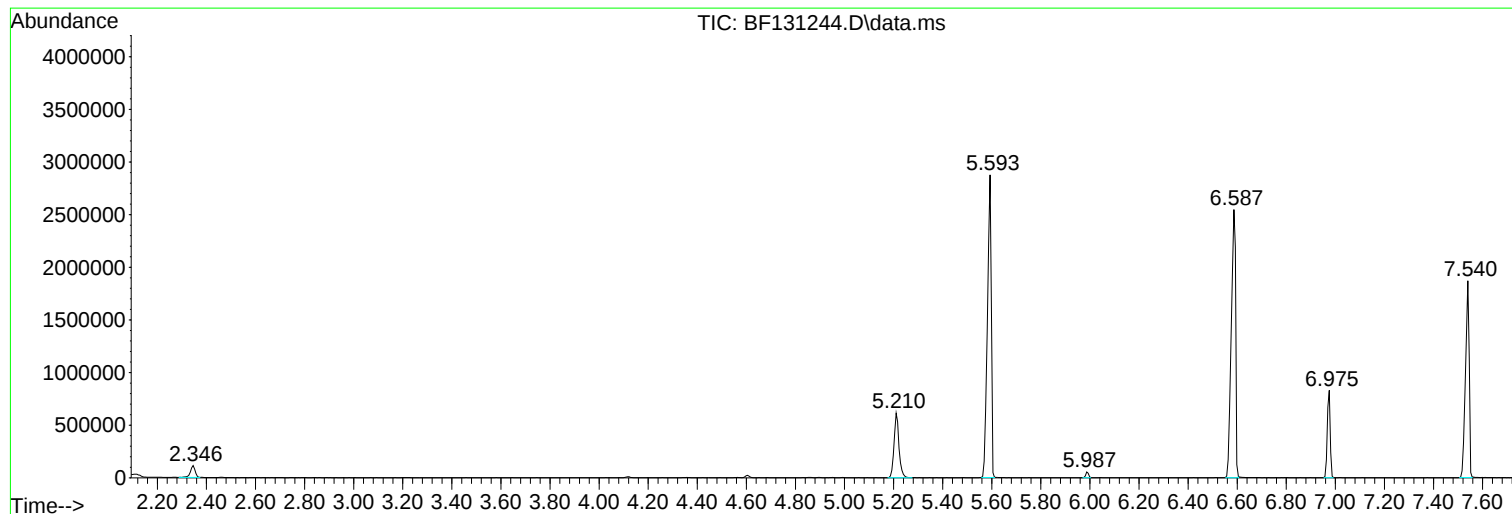
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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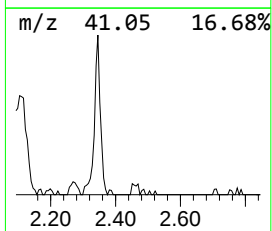
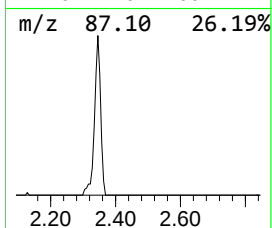
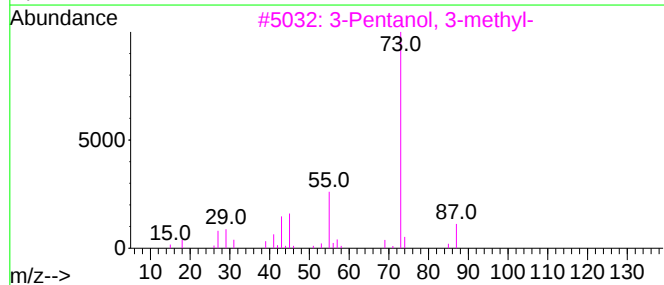
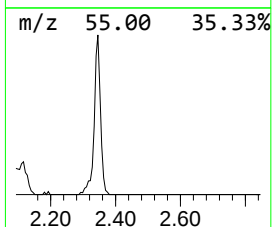
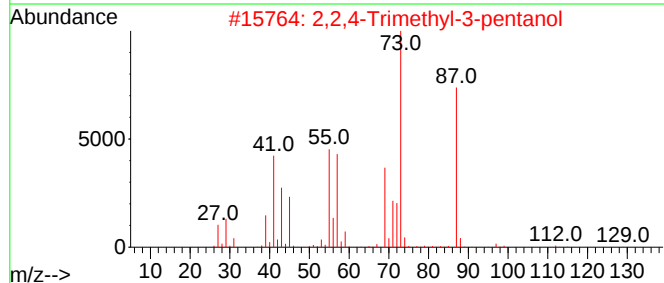
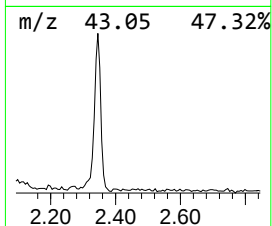
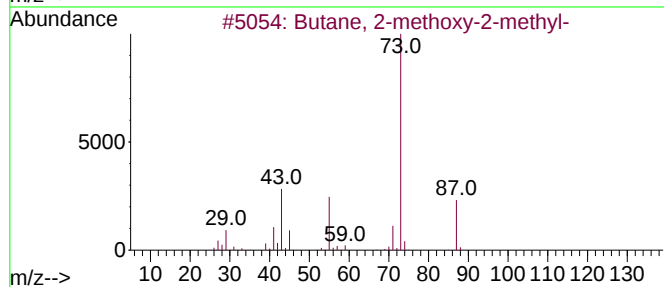
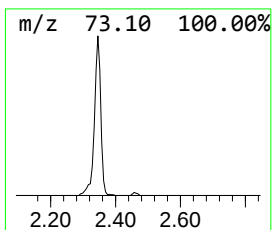
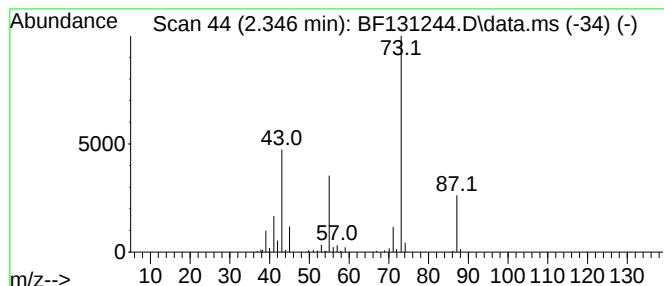
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.346	4.37 ng	149161	1,4-Dichlorobenzene-d4	6.975

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	40
3			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	28
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25



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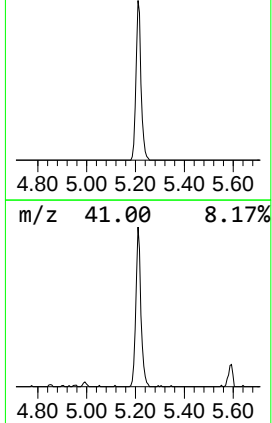
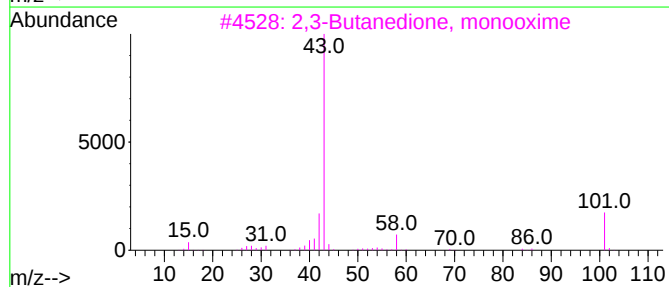
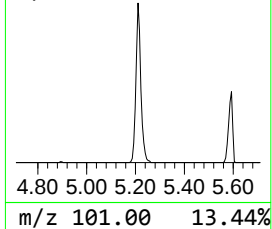
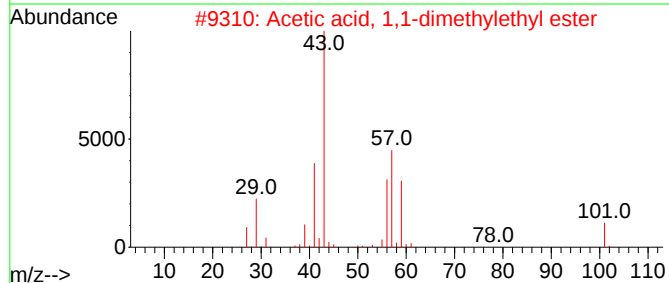
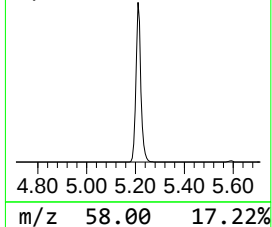
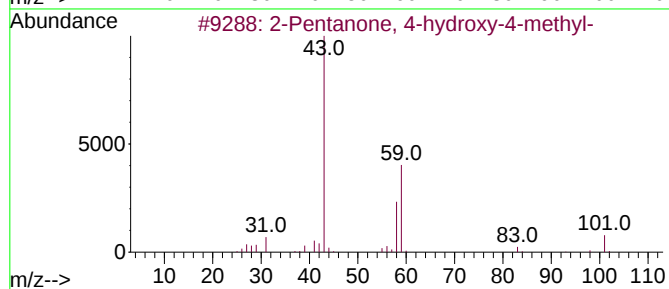
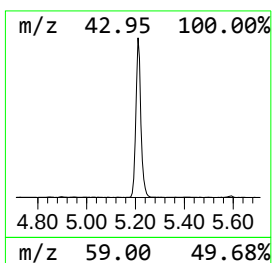
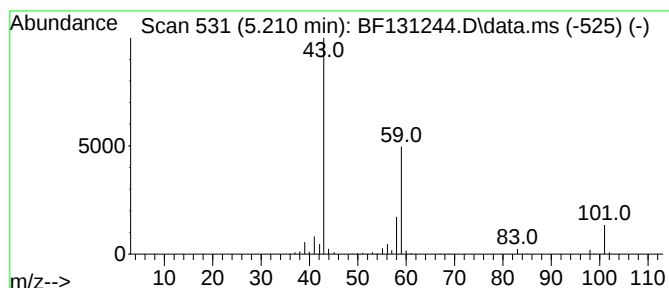
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.210	24.95 ng	851772	1,4-Dichlorobenzene-d4	6.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Allyl acetate	100	C5H8O2	000591-87-7	9



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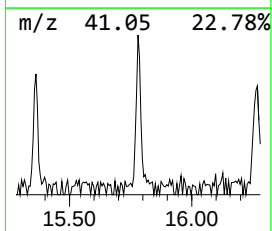
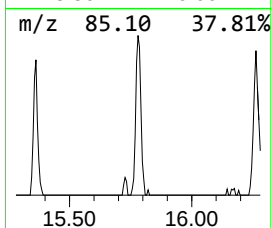
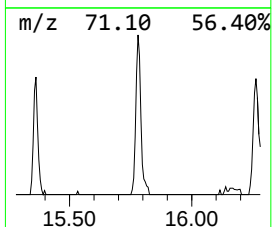
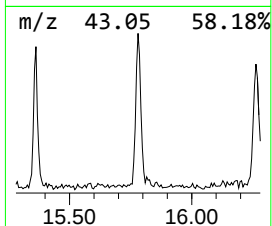
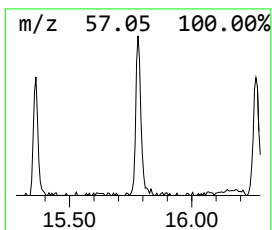
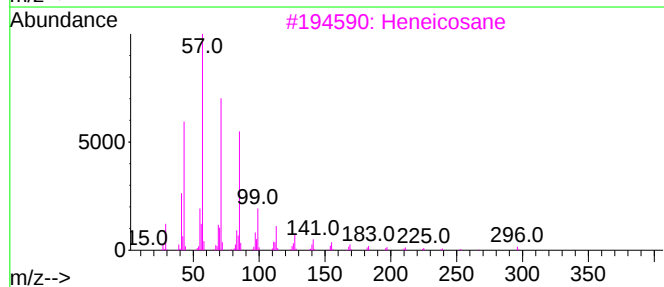
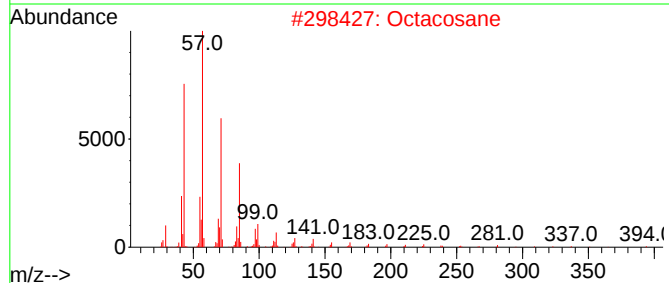
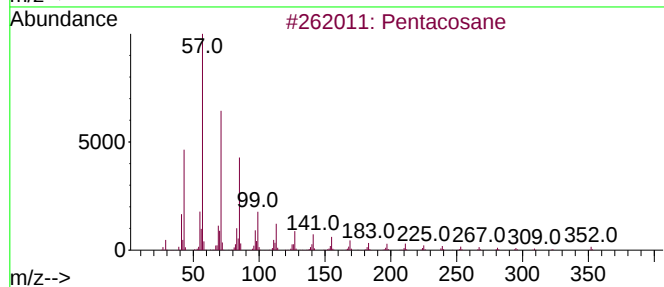
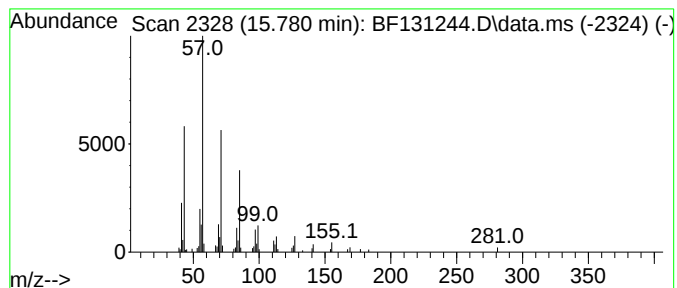
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Peak Number 3 Pentacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.780	2.09 ng	83822	Perylene-d12	15.727

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	91
2			Octacosane	394	C28H58	000630-02-4	90
3			Heneicosane	296	C21H44	000629-94-7	87
4			Heptacosane	380	C27H56	000593-49-7	87
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	87



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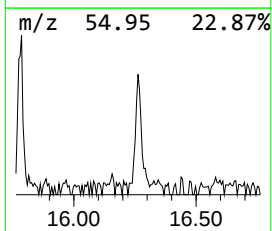
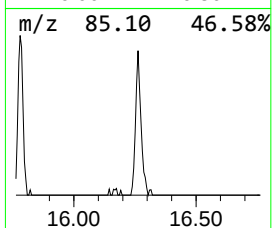
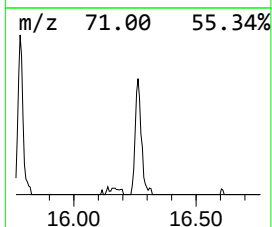
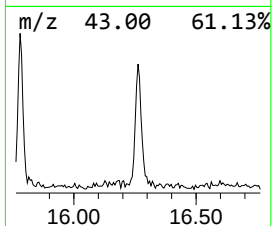
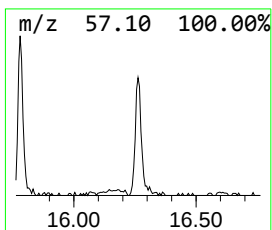
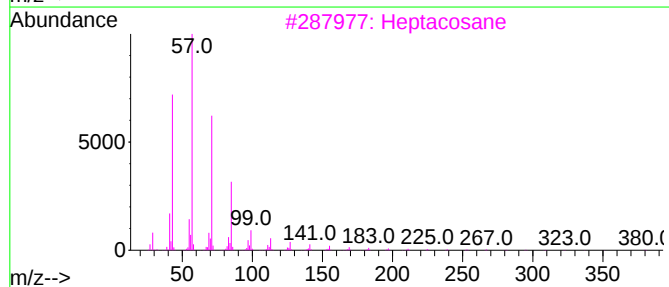
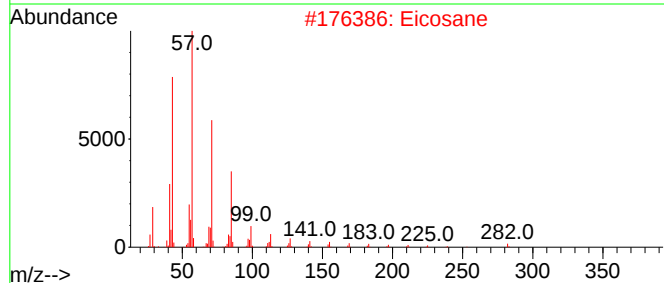
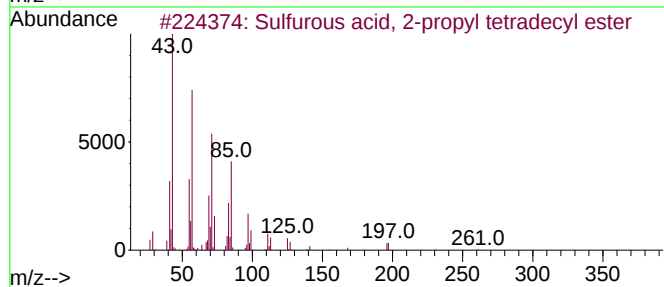
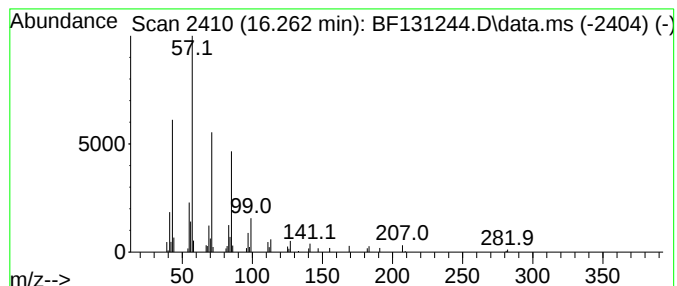
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Peak Number 4 Sulfurous acid, 2-propyl te... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.262	2.00 ng	80432	Perylene-d12	15.727

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-propyl tetradecyl ester	320	C17H36O3S	1010309-12-5	78
2			Eicosane	282	C20H42	000112-95-8	76
3			Heptacosane	380	C27H56	000593-49-7	72
4			Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	64
5			Borane, diethyl(decyloxy)-	226	C14H31BO	1000152-34-3	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.346	4.4	ng	149161	1	6.975	682772	20.0
2-Pentanone, 4-...	5.210	24.9	ng	851772	1	6.975	682772	20.0
Pentacosane	15.780	2.1	ng	83822	6	15.727	803996	20.0
Sulfurous acid,...	16.262	2.0	ng	80432	6	15.727	803996	20.0