

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120722\
 Data File : BF131549.D
 Acq On : 07 Dec 2022 22:50
 Operator : CG\JU
 Sample : PB149277BL
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB149277BL

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-BF120722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131549.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	16	23	28	rVB	45330	58248	1.37%	0.285%
2	5.134	513	518	529	rBV	288878	428061	10.09%	2.091%
3	5.528	579	585	588	rBV	2253628	2251800	53.07%	11.002%
4	6.534	750	756	759	rBV	1995757	2336524	55.07%	11.416%
5	6.904	816	819	823	rBV	465181	416485	9.82%	2.035%
6	7.481	910	917	919	rBV	1326061	1538244	36.25%	7.516%
7	8.198	1034	1039	1042	rBV	618640	546896	12.89%	2.672%
8	9.281	1217	1223	1226	rBV	3635890	3170879	74.73%	15.493%
9	9.963	1333	1339	1342	rBV	817161	714532	16.84%	3.491%
10	10.757	1467	1474	1477	rBV	2684460	2363504	55.70%	11.548%
11	11.457	1589	1593	1596	rVB	934604	811703	19.13%	3.966%
12	13.057	1859	1865	1867	rBV	4167816	4243022	100.00%	20.731%
13	14.104	2039	2043	2047	rBV	799876	664934	15.67%	3.249%
14	15.245	2231	2237	2243	rBV	47763	55669	1.31%	0.272%
15	15.616	2294	2300	2311	rBV	375809	567914	13.38%	2.775%
16	16.104	2377	2383	2390	rBV2	46737	76566	1.80%	0.374%
17	16.633	2468	2473	2482	rBV2	38232	68838	1.62%	0.336%
18	17.262	2574	2580	2591	rBV2	23736	52709	1.24%	0.258%
19	17.580	2620	2634	2636	rBV4	17872	57536	1.36%	0.281%
20	18.015	2698	2708	2715	rBV5	15599	42897	1.01%	0.210%

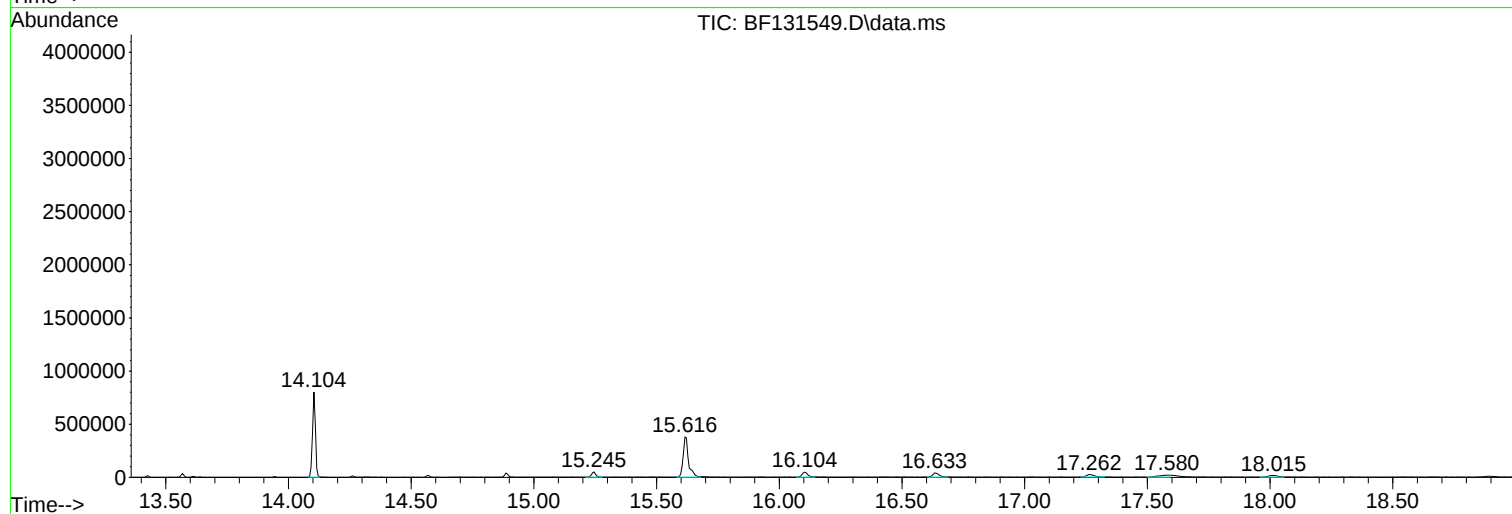
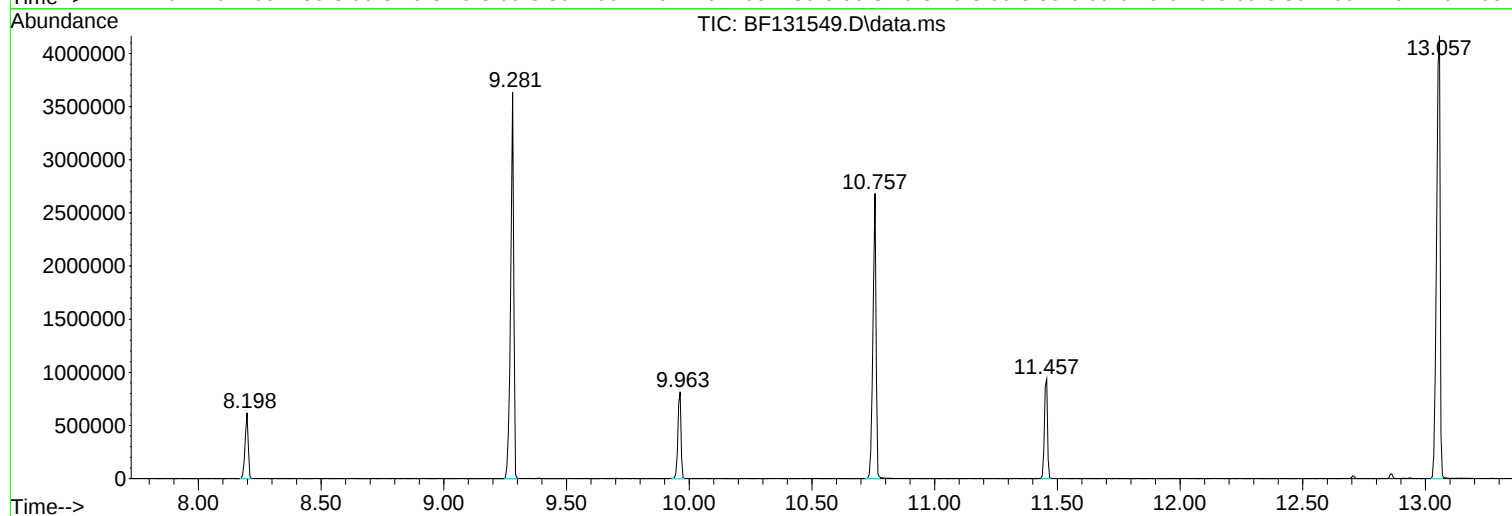
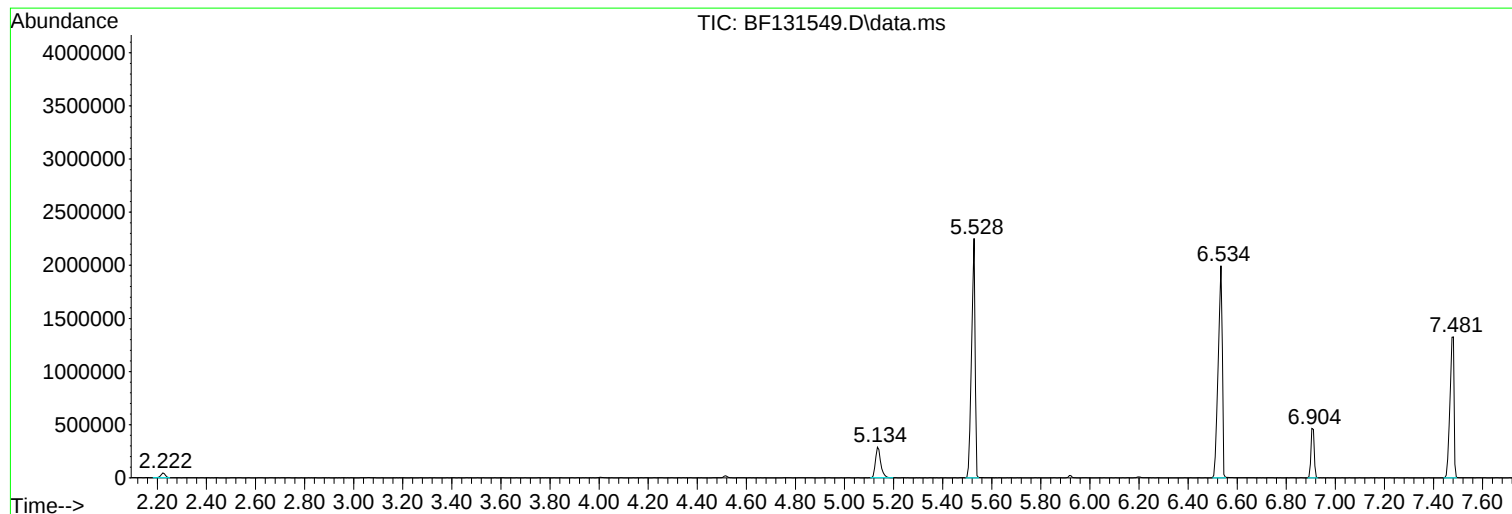
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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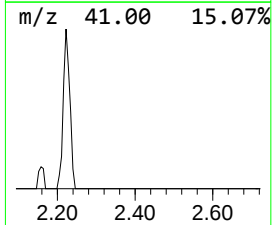
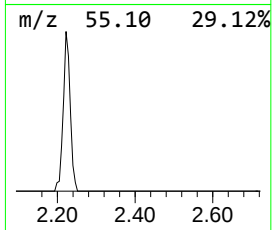
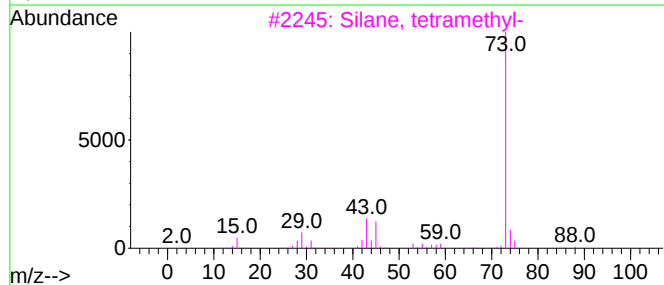
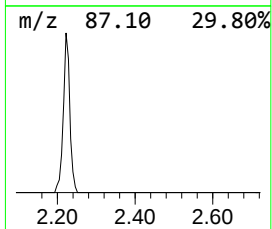
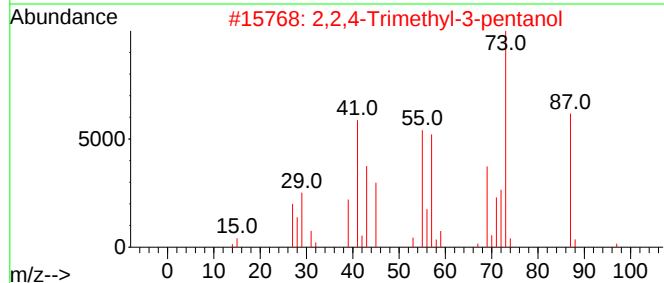
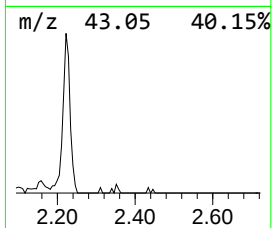
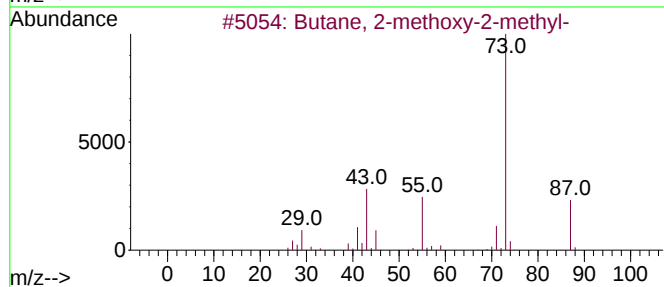
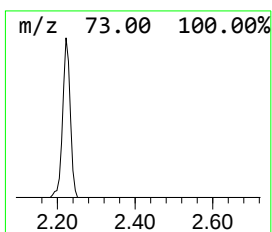
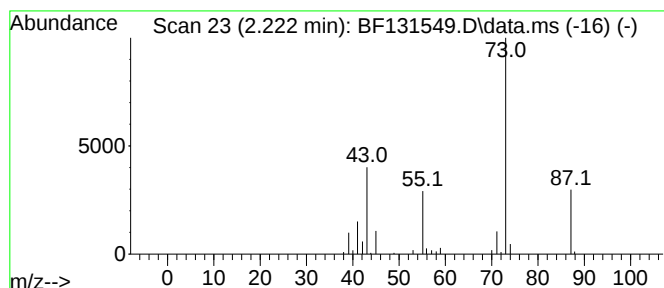
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.222	2.80 ng	58248	1,4-Dichlorobenzene-d4	6.910

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	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	27
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	17



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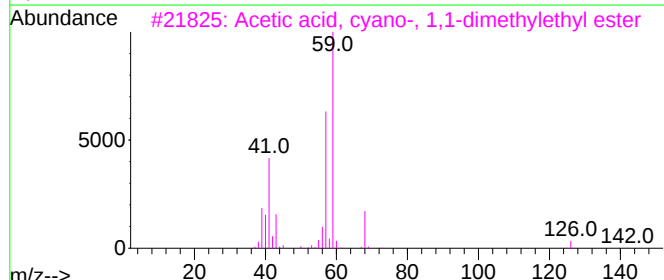
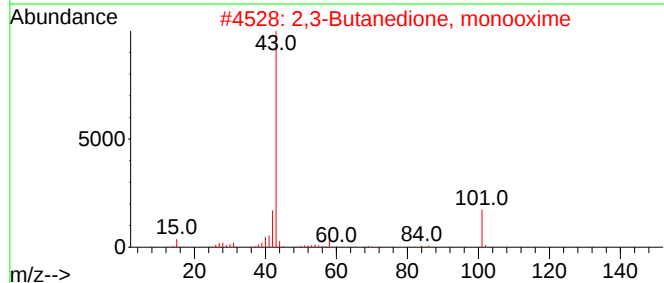
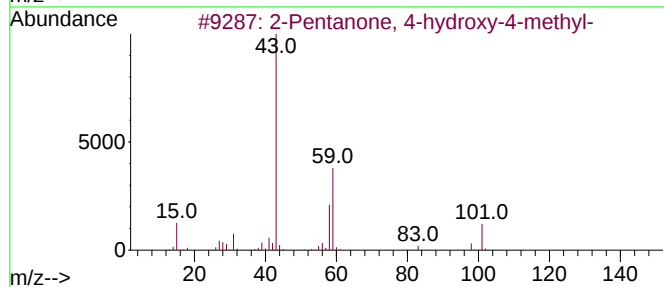
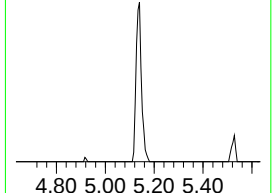
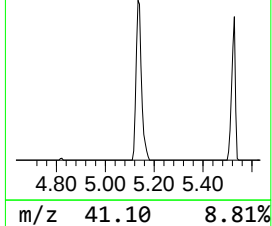
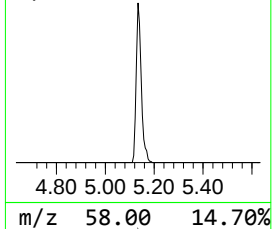
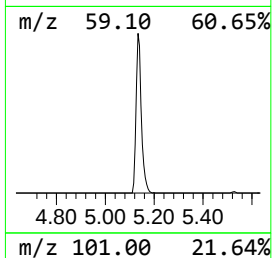
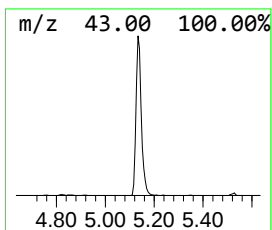
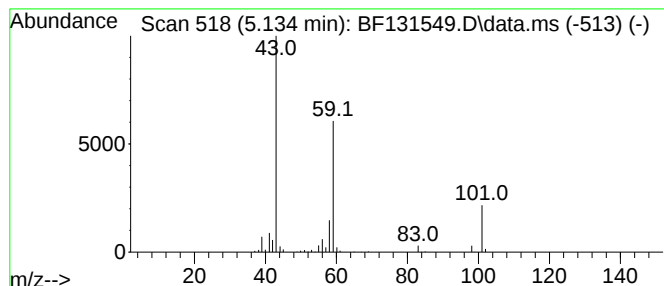
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120722.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.134	20.56 ng	428061	1,4-Dichlorobenzene-d4			6.910
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	35
3	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	32
4	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	9



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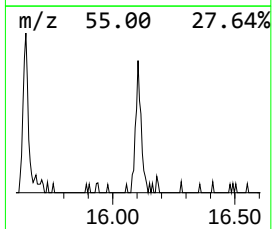
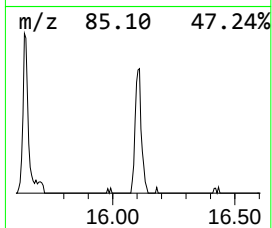
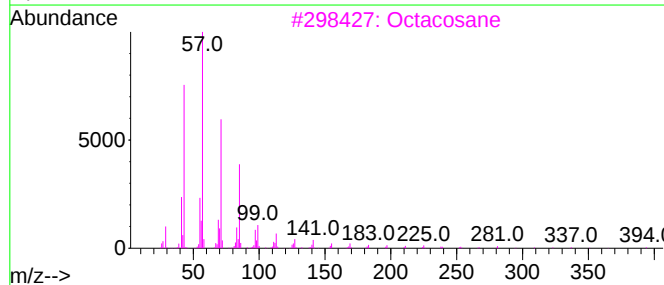
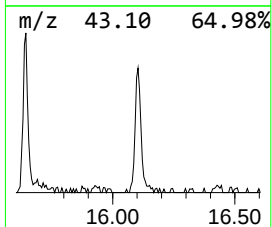
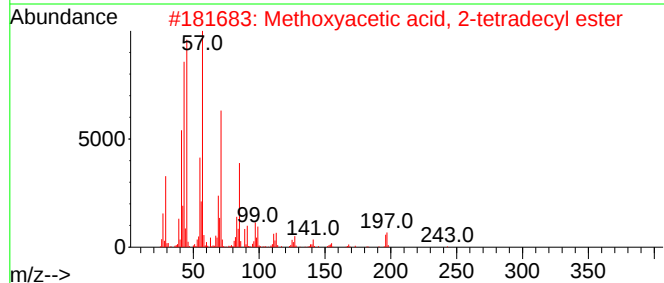
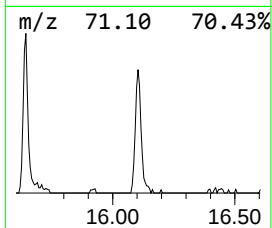
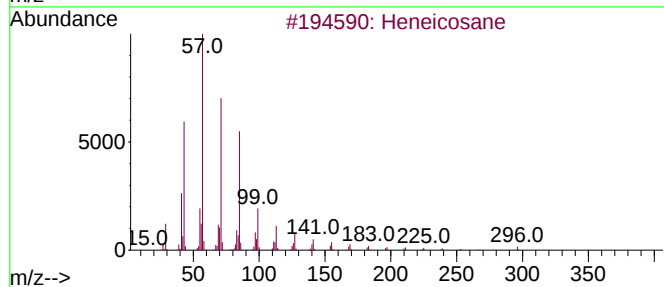
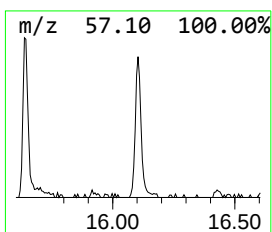
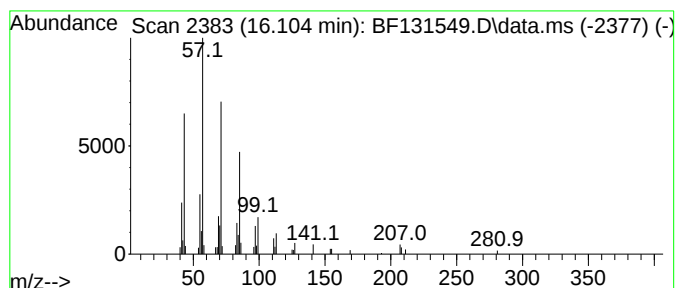
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.104	2.70 ng	76566	Perylene-d12	15.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	87
2			Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	87
3			Octacosane	394	C28H58	000630-02-4	87
4			Hexacosane	366	C26H54	000630-01-3	87
5			Octadecane, 2-methyl-	268	C19H40	001560-88-9	86



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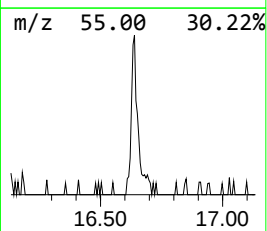
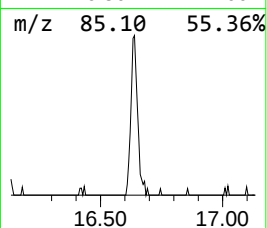
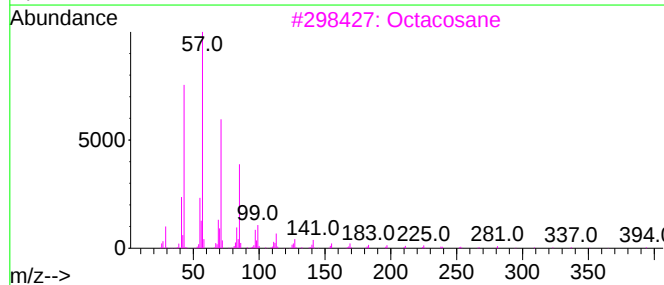
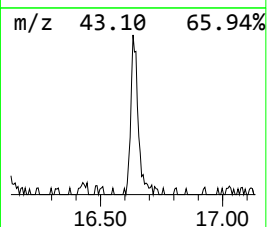
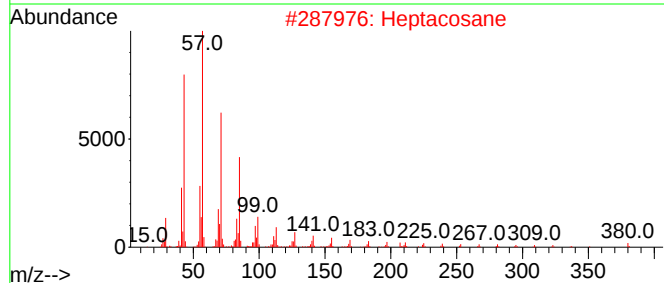
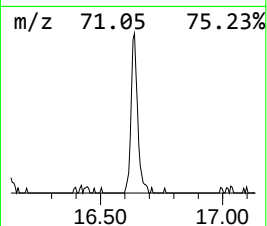
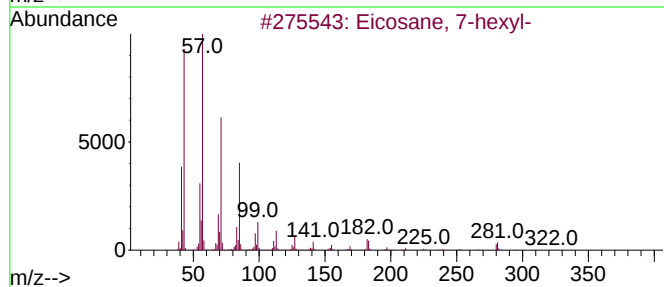
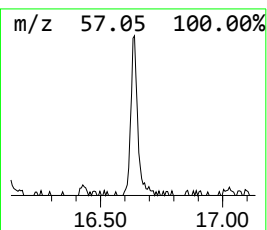
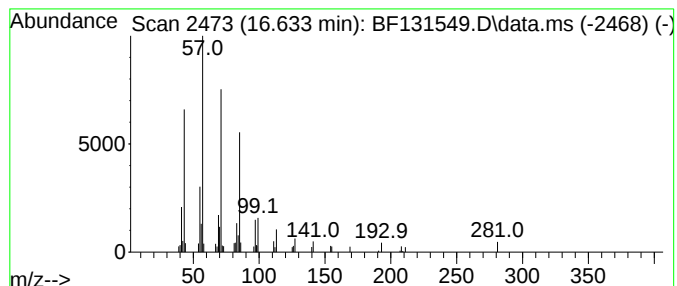
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Peak Number 4 Eicosane, 7-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.633	2.42 ng	68838	Perylene-d12	15.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
2			Heptacosane	380	C27H56	000593-49-7	90
3			Octacosane	394	C28H58	000630-02-4	87
4			Heptadecane	240	C17H36	000629-78-7	87
5			Hexacosane	366	C26H54	000630-01-3	86



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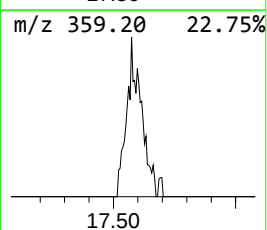
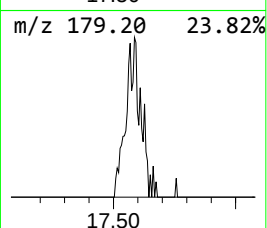
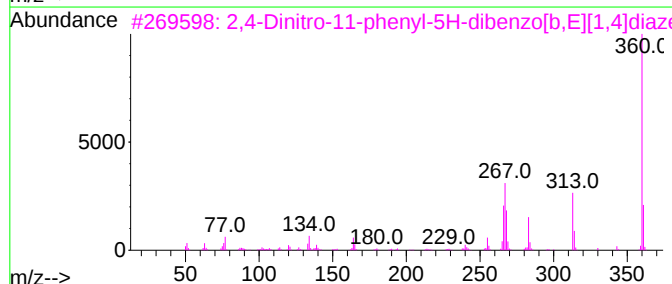
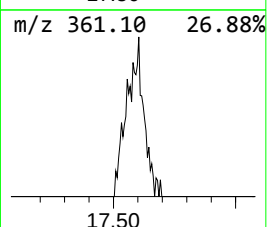
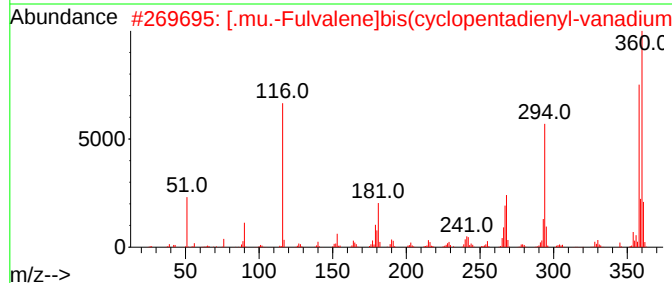
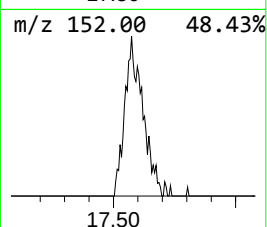
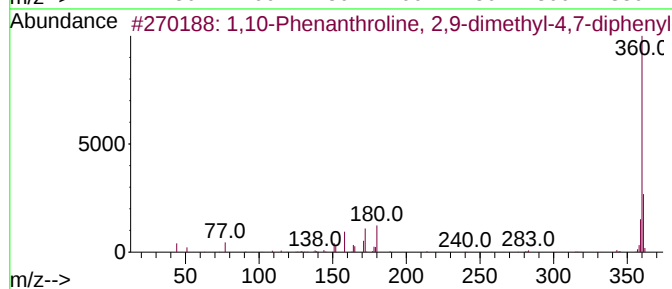
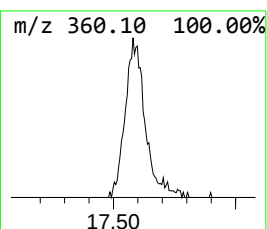
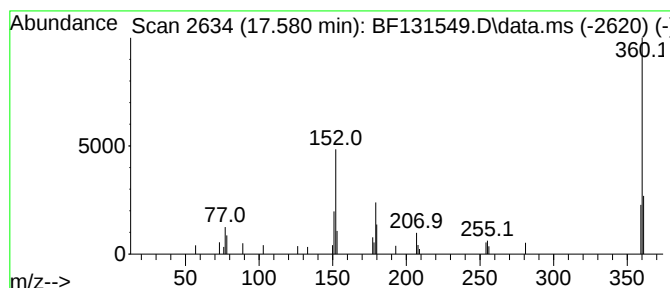
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown17.580 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.580	2.03 ng	57536	Perylene-d12	15.616

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	38
2		[.mu.-Fulvalene]bis(cyclopentadi...	360	C20H18V2	1000163-45-2	37
3		2,4-Dinitro-11-phenyl-5H-dibenzo...	360	C19H12N4O4	071354-26-2	25
4		3.beta.-N-Methylacetamido-17-ami...	360	C23H40N2O	1010280-91-0	17
5		Pentacyclo[18.4.1.1(2,7).1(8,13)...	360	C28H24	101077-60-5	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.222	2.8	ng	58248	1	6.910	416485	20.0
2-Pentanone, 4-...	5.134	20.6	ng	428061	1	6.910	416485	20.0
Heneicosane	16.104	2.7	ng	76566	6	15.616	567914	20.0
Eicosane, 7-hexyl-	16.633	2.4	ng	68838	6	15.616	567914	20.0
unknown17.580	17.580	2.0	ng	57536	6	15.616	567914	20.0