

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122322\
 Data File : BF131806.D
 Acq On : 23 Dec 2022 14:58
 Operator : CG\JU
 Sample : PB149846BL
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB149846BL

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-BF122022.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131806.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	10	18	rVB	86788	112608	2.31%	0.454%
2	5.069	500	507	521	rBV	129490	212942	4.36%	0.859%
3	5.469	570	575	578	rBV	2673903	2687535	55.05%	10.842%
4	6.481	742	747	750	rBV	2337918	2755242	56.43%	11.115%
5	6.845	806	809	813	rBV	730962	584839	11.98%	2.359%
6	7.416	901	906	909	rBV	1620343	1829711	37.48%	7.382%
7	8.139	1024	1029	1032	rBV	831824	786549	16.11%	3.173%
8	9.222	1207	1213	1216	rBV	3532197	3683366	75.44%	14.860%
9	9.904	1323	1329	1332	rBV	1215321	1015202	20.79%	4.096%
10	10.704	1458	1465	1468	rBV	2855826	2608048	53.42%	10.522%
11	11.404	1578	1584	1587	rBV	1421635	1181084	24.19%	4.765%
12	12.816	1820	1824	1827	rBV	122171	104671	2.14%	0.422%
13	13.004	1851	1856	1859	rBV	4787966	4882367	100.00%	19.697%
14	13.521	1941	1944	1948	rBV	87864	70883	1.45%	0.286%
15	14.062	2031	2036	2039	rBV	1149472	1026614	21.03%	4.142%
16	14.839	2164	2168	2171	rVB	50815	51056	1.05%	0.206%
17	15.186	2223	2227	2231	rVB	61414	67157	1.38%	0.271%
18	15.562	2285	2291	2299	rVB	556786	795139	16.29%	3.208%
19	16.027	2365	2370	2376	rVB	60304	94712	1.94%	0.382%
20	16.551	2453	2459	2466	rBV	53114	97991	2.01%	0.395%
21	17.162	2557	2563	2570	rBV2	33005	66960	1.37%	0.270%
22	17.892	2678	2687	2695	rBV3	27383	72897	1.49%	0.294%

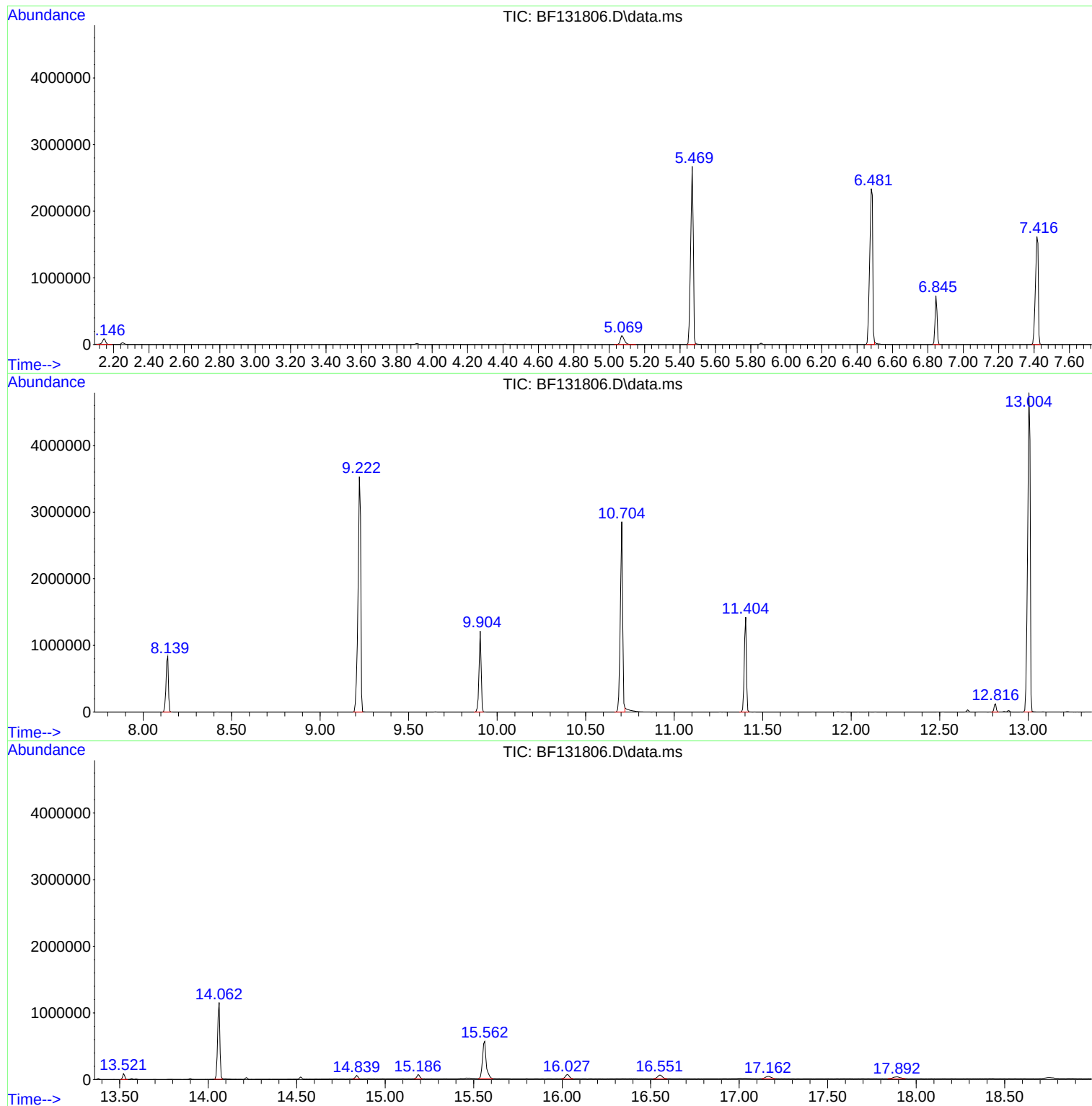
Sum of corrected areas: 24787573

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.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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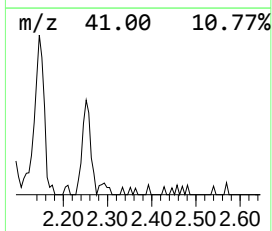
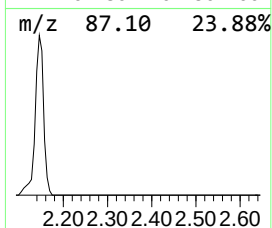
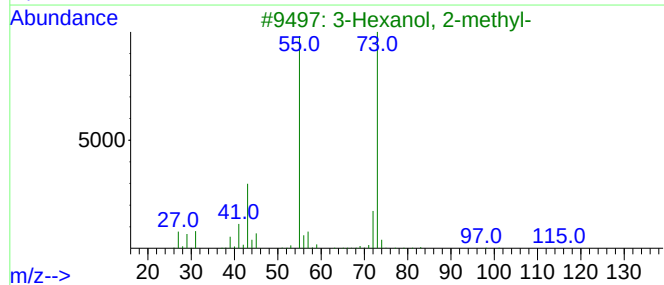
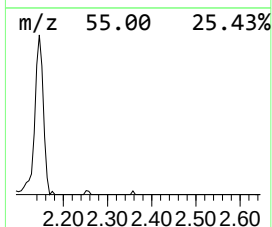
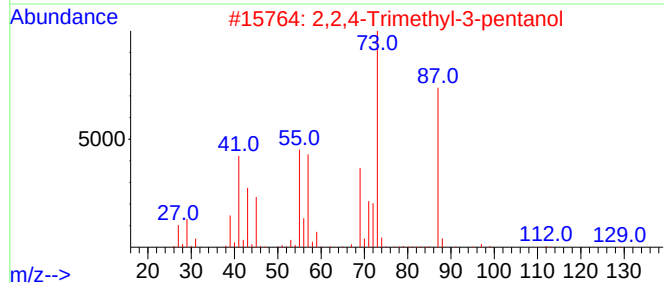
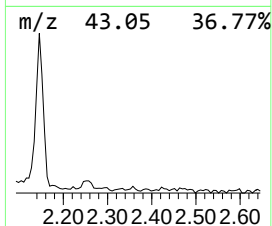
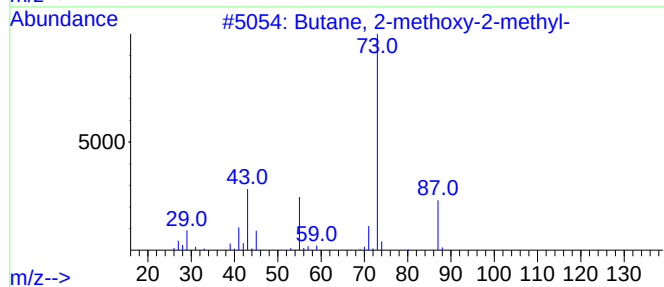
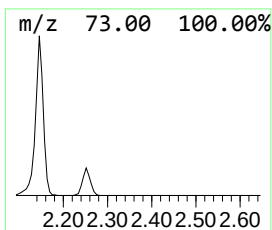
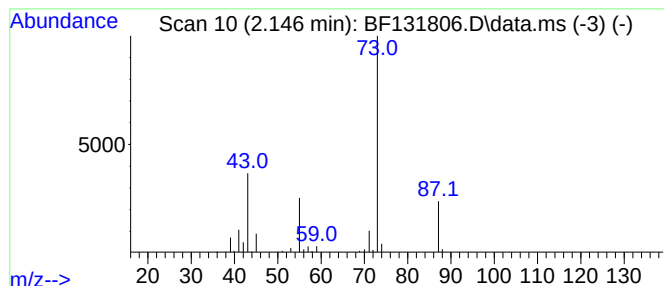
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.146	3.85 ng	112608	1,4-Dichlorobenzene-d4	6.845

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			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
4			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10



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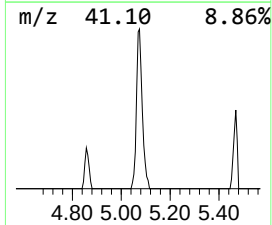
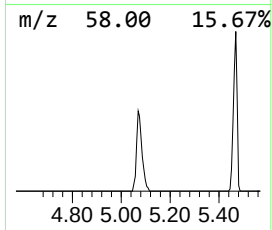
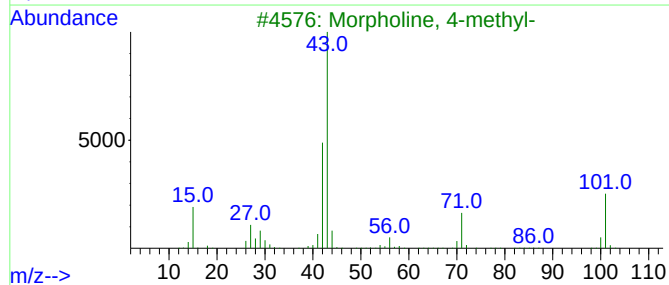
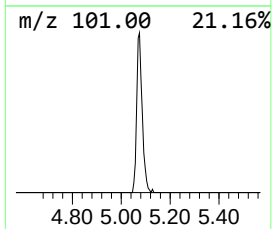
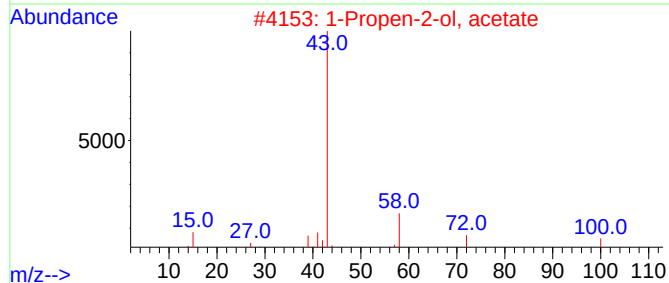
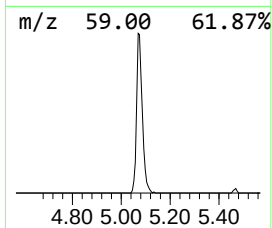
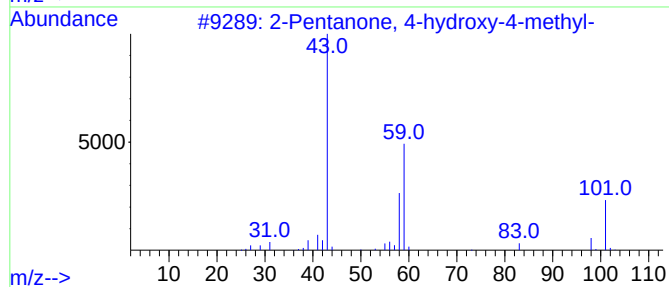
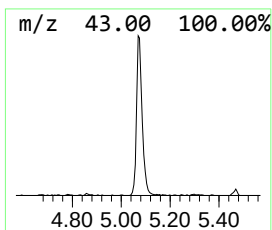
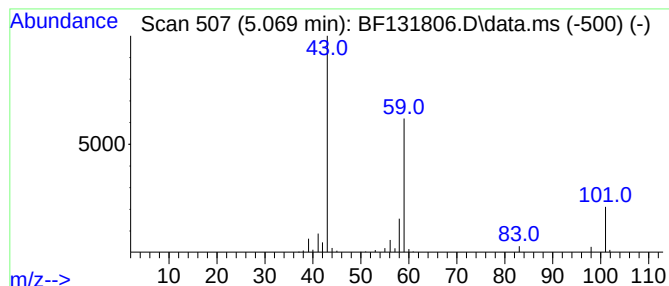
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.069	7.28 ng	212942	1,4-Dichlorobenzene-d4			6.845
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	72
2	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	10
3	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	9
4	4-Penten-2-one, 4-methyl-		98	C6H10O	003744-02-3	9
5	Butane, 1-ethoxy-		102	C6H14O	000628-81-9	9



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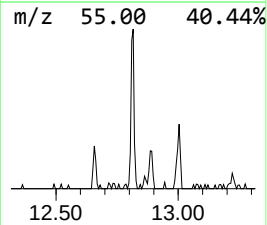
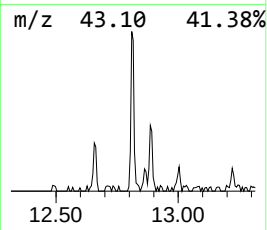
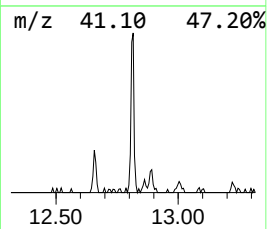
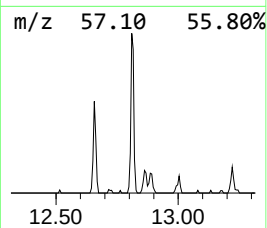
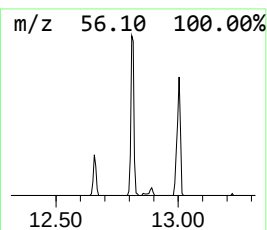
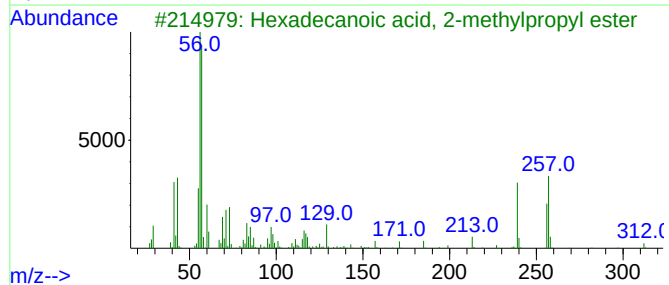
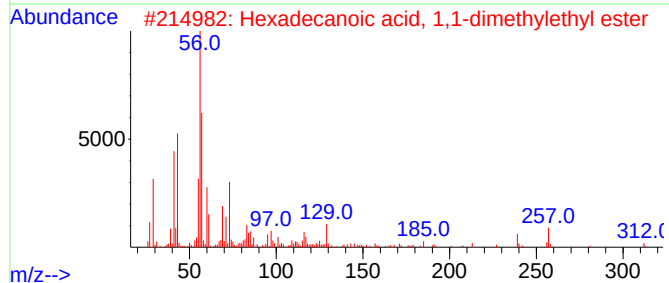
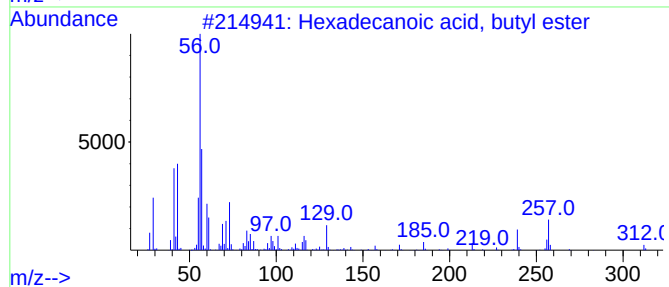
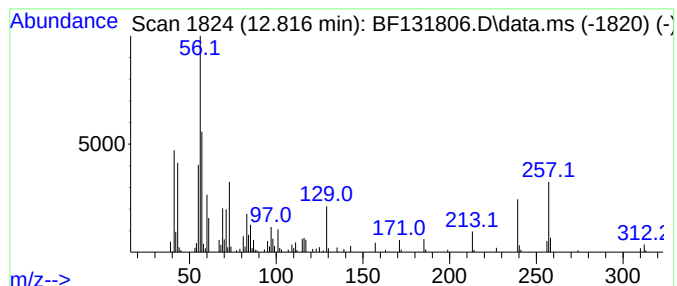
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Peak Number 3 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.816	2.04 ng	104671	Chrysene-d12	14.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	97
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	96
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	76
4	Nipecotic acid	129	C6H11NO2	000498-95-3	43
5	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	25



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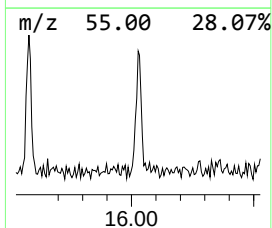
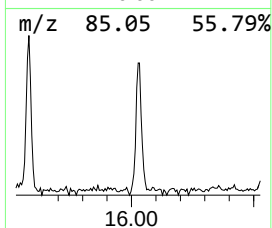
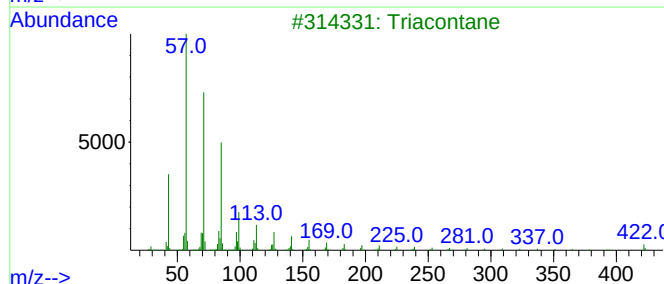
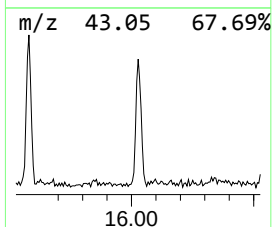
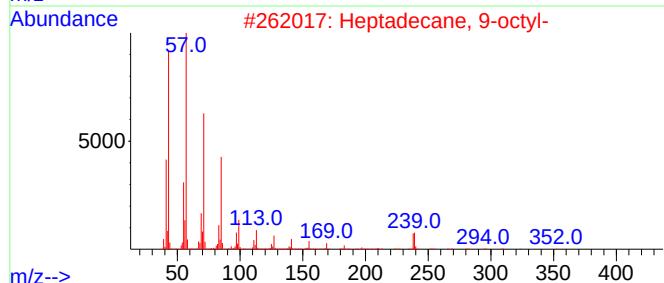
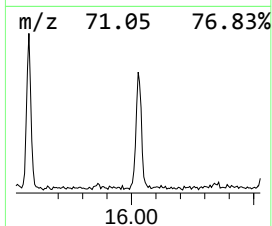
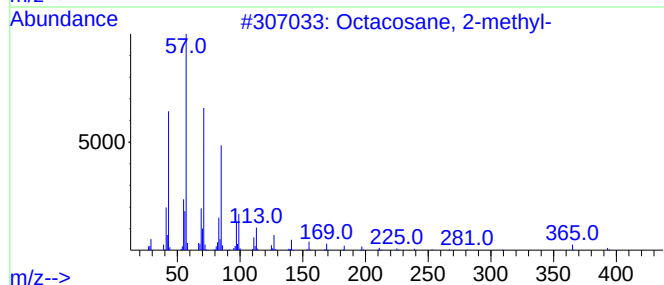
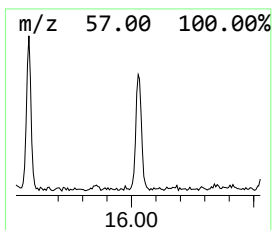
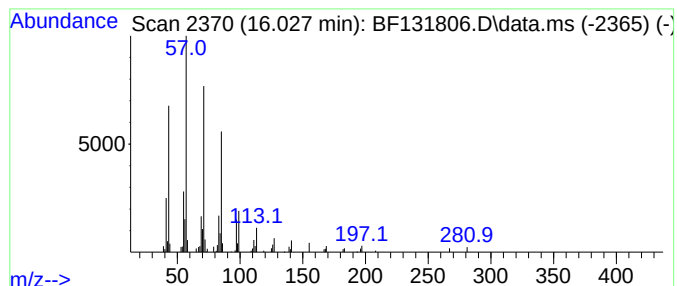
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octacosane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.027	2.38 ng	94712	Perylene-d12	15.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3			Triacontane	422	C30H62	000638-68-6	91
4			Heneicosane	296	C21H44	000629-94-7	91
5			Hexacosane	366	C26H54	000630-01-3	90



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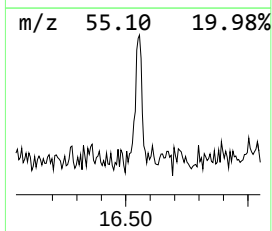
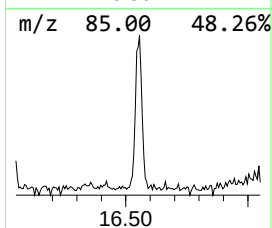
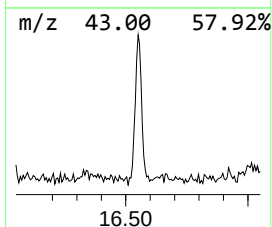
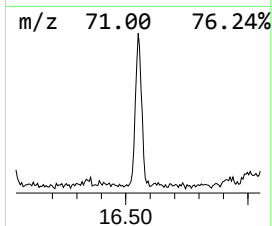
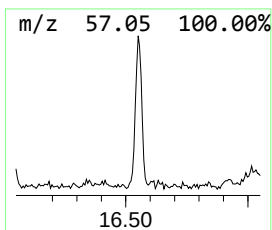
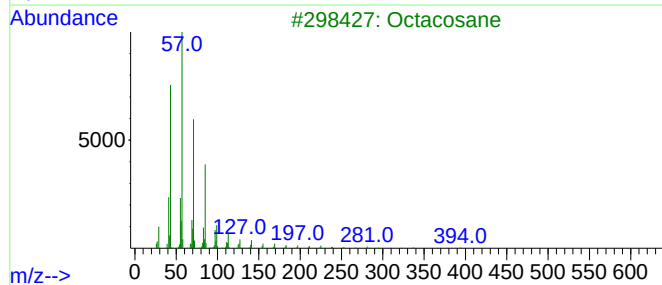
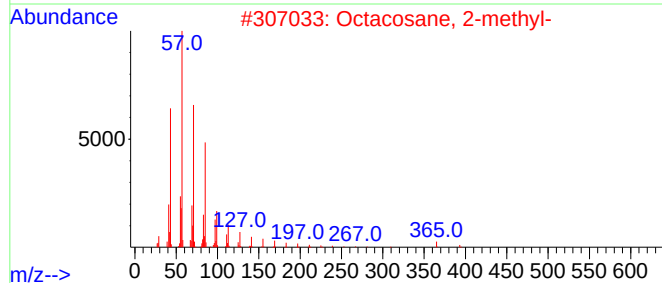
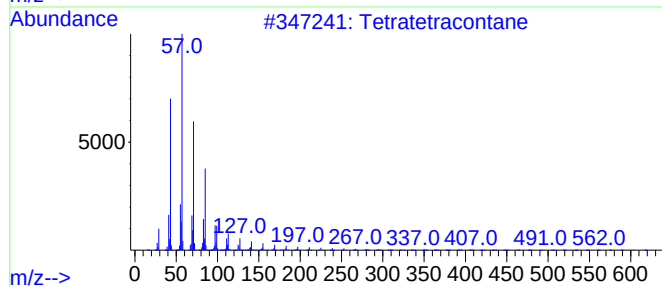
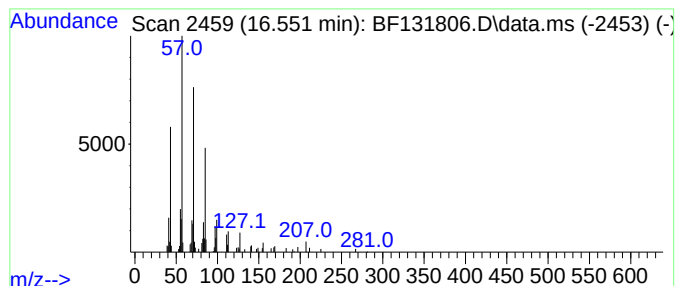
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Tetratetracontane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.551	2.46 ng	97991	Perylene-d12	15.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Hexacosane	366	C26H54	000630-01-3	91
5			Hentriacontane	437	C31H64	000630-04-6	91



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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...	2.146	3.9	ng	112608	1	6.845	584839	20.0
2-Pentanone, 4-...	5.069	7.3	ng	212942	1	6.845	584839	20.0
Hexadecanoic ac...	12.816	2.0	ng	104671	5	14.063	1026610	20.0
Octacosane, 2-m...	16.027	2.4	ng	94712	6	15.562	795139	20.0
Tetratetracontane	16.551	2.5	ng	97991	6	15.562	795139	20.0