

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071824\
 Data File : BM046715.D
 Acq On : 18 Jul 2024 23:21
 Operator : MA/JU
 Sample : P3246-16
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 WC-CTW2-BL-04

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_M\Methods\8270-BM071724.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM046715.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.358	60	63	68	rBV	70270	82366	2.58%	0.375%
2	4.681	283	288	296	rVB	91520	124533	3.91%	0.567%
3	5.128	356	364	372	rBV	1431633	1938902	60.81%	8.826%
4	6.687	621	629	639	rVB	1477811	2168107	68.00%	9.870%
5	7.487	757	765	772	rVB	426314	665772	20.88%	3.031%
6	8.628	947	959	966	rBV	897480	1425155	44.70%	6.488%
7	10.245	1226	1234	1242	rBV	535627	865947	27.16%	3.942%
8	10.998	1356	1362	1370	rBV	43746	77381	2.43%	0.352%
9	12.745	1652	1659	1666	rBV	2181087	3129783	98.16%	14.248%
10	14.133	1887	1895	1901	rBV	796149	1181682	37.06%	5.379%
11	14.363	1928	1934	1935	rBV4	30383	34453	1.08%	0.157%
12	14.386	1935	1938	1946	rVB6	36846	74243	2.33%	0.338%
13	15.627	2139	2149	2157	rBV	2024465	2727255	85.53%	12.415%
14	16.886	2357	2363	2368	rBV	907143	1282797	40.23%	5.840%
15	17.821	2516	2522	2528	rBV	258476	369047	11.57%	1.680%
16	18.951	2711	2714	2720	rVB	39689	51277	1.61%	0.233%
17	19.027	2723	2727	2730	rBV4	30140	40248	1.26%	0.183%
18	19.109	2737	2741	2753	rBV	98505	164407	5.16%	0.748%
19	19.315	2773	2776	2779	rVB	33803	38959	1.22%	0.177%
20	19.539	2808	2814	2821	rBV	2702263	3188555	100.00%	14.515%
21	19.704	2839	2842	2847	rBV4	25827	32446	1.02%	0.148%
22	20.851	3033	3037	3043	rVB2	149137	209946	6.58%	0.956%
23	21.056	3070	3072	3076	rBV2	39757	50609	1.59%	0.230%
24	21.109	3076	3081	3086	rVV	752071	984441	30.87%	4.481%
25	23.874	3544	3551	3559	rVB	483483	1058571	33.20%	4.819%

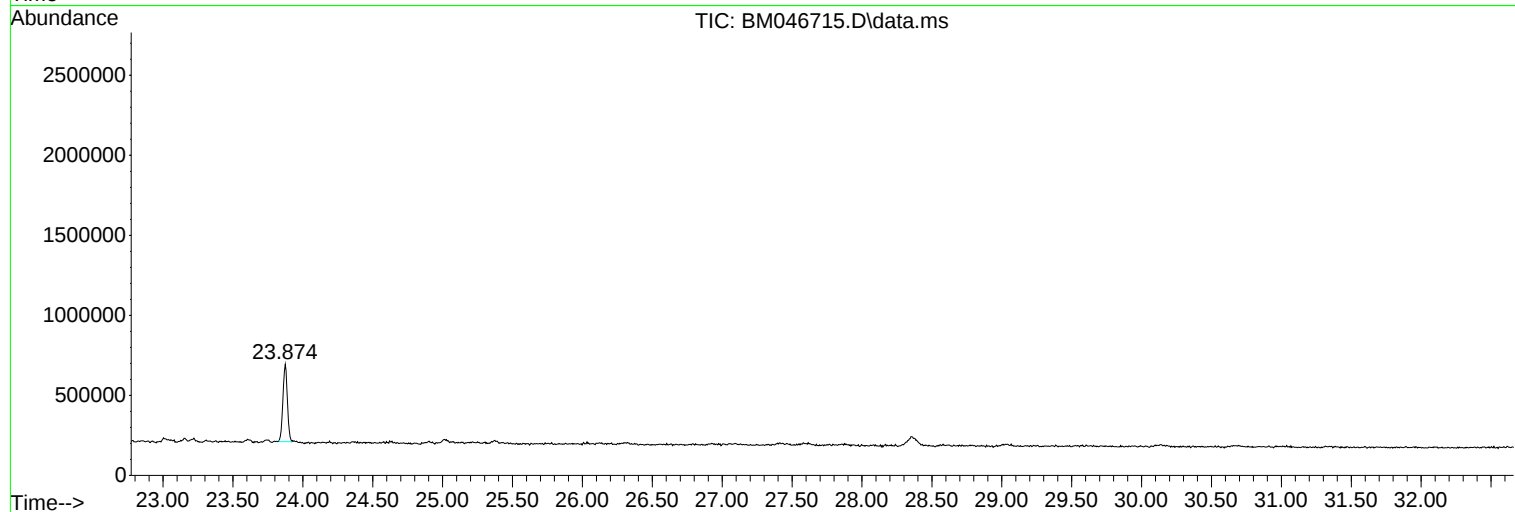
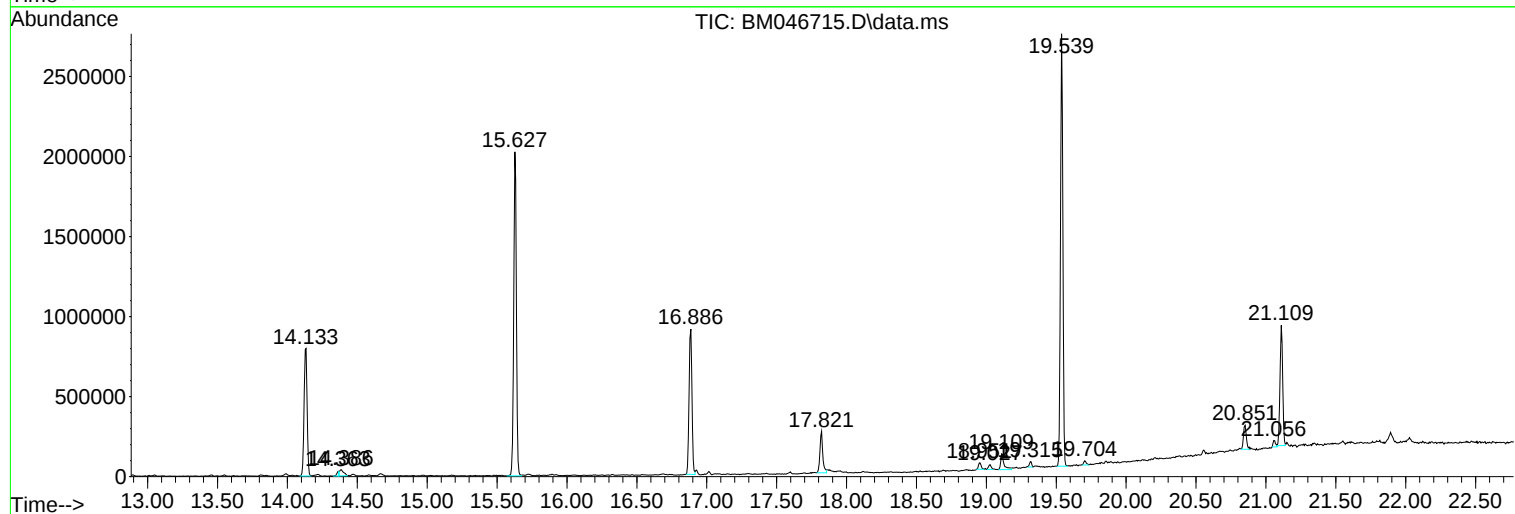
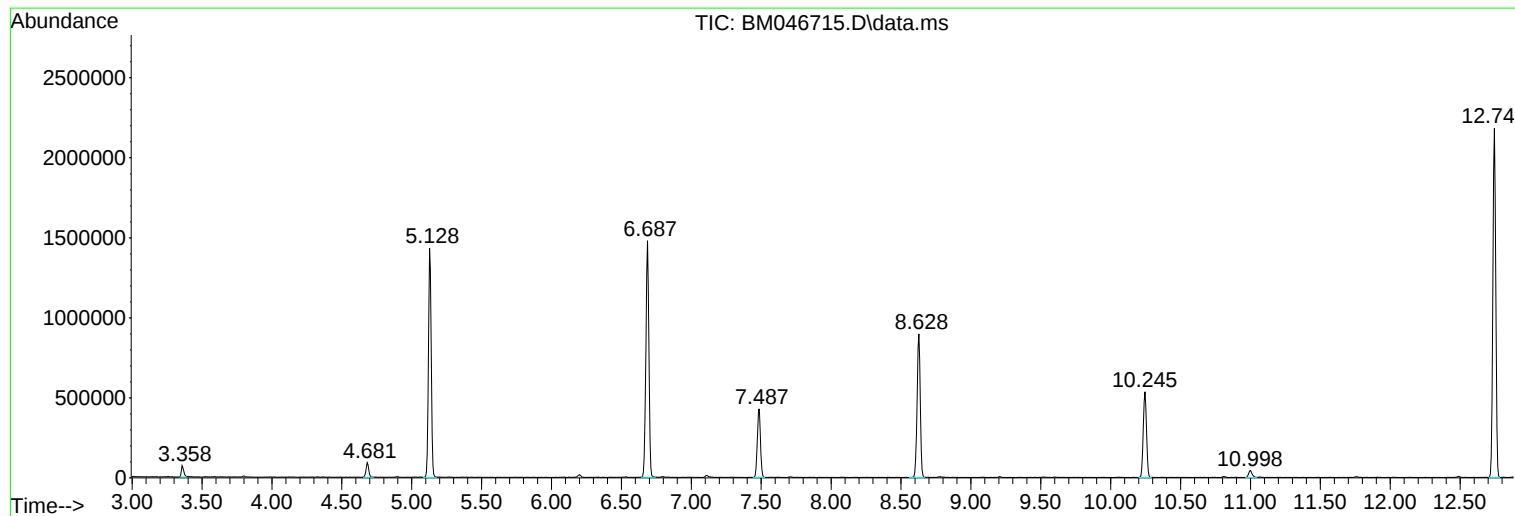
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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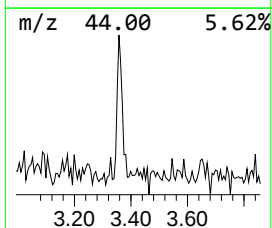
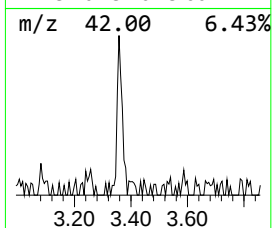
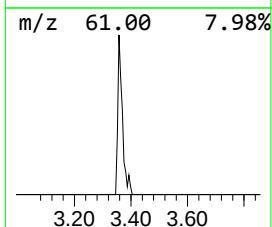
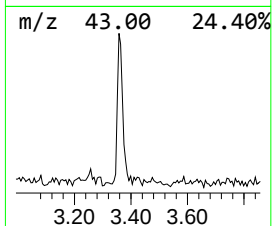
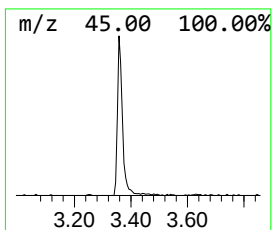
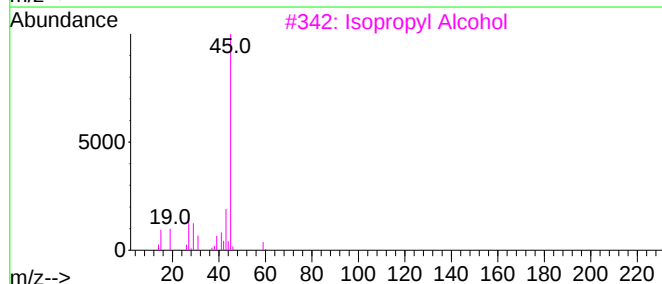
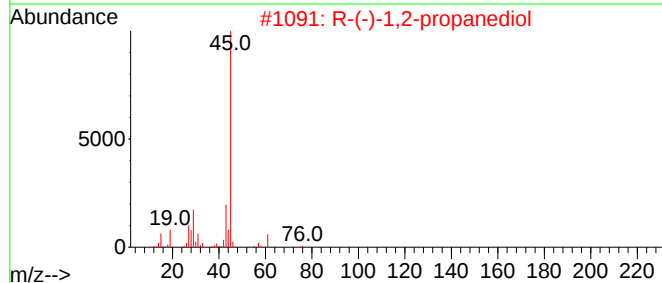
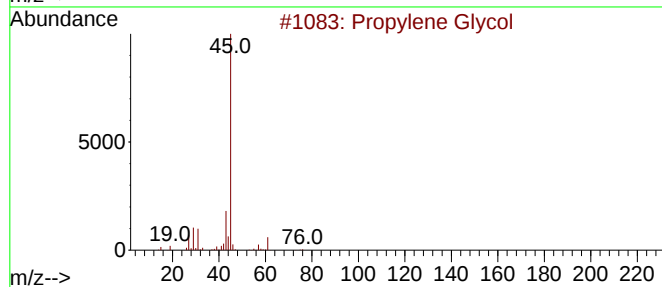
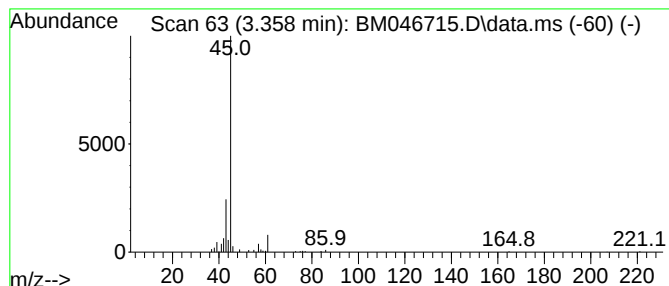
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.358	2.47 ng	82366	1,4-Dichlorobenzene-d4	7.487

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propylene Glycol	76	C3H8O2	000057-55-6	80
2		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
3		Isopropyl Alcohol	60	C3H8O	000067-63-0	50
4		2,4-Pentanediol	104	C5H12O2	000625-69-4	38
5		2-Octanol, (S)-	130	C8H18O	006169-06-8	9



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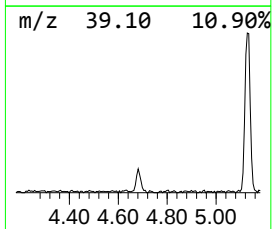
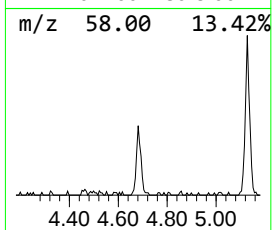
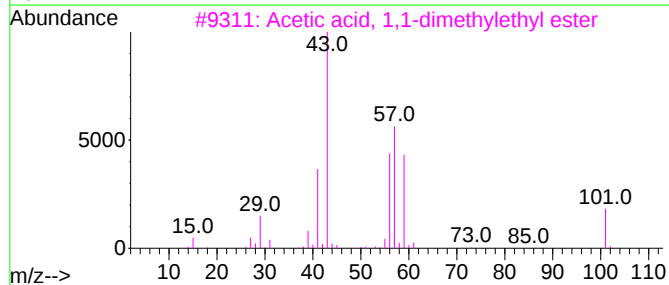
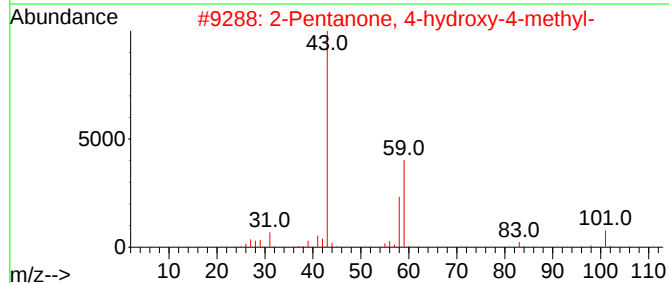
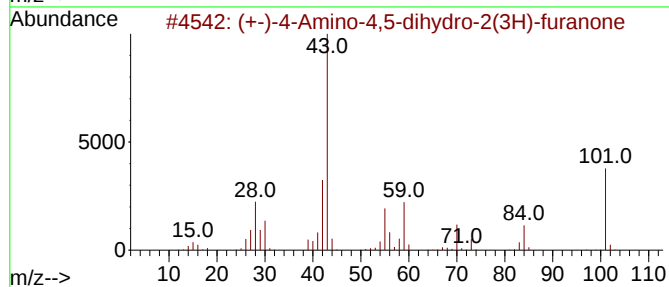
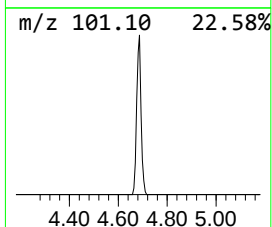
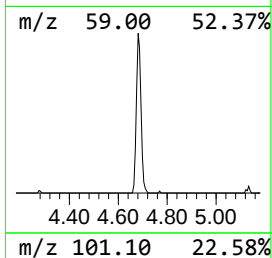
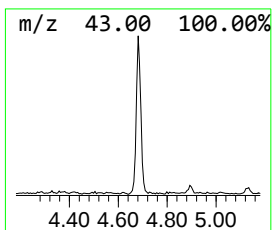
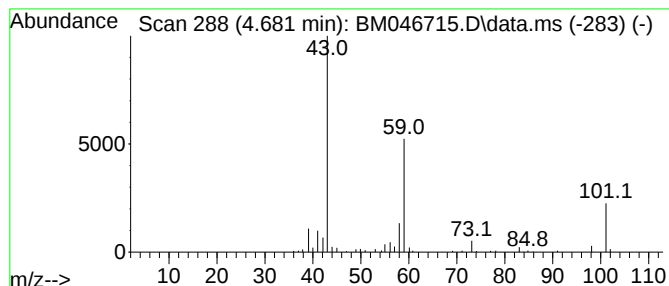
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (+)-4-Amino-4,5-dihydro-2(...) Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.681	3.74 ng	124533	1,4-Dichlorobenzene-d4	7.487

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	72
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	45
4		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	38
5		Silane, trimethyl-	74	C3H10Si	000993-07-7	38



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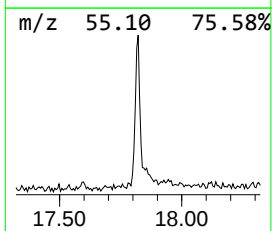
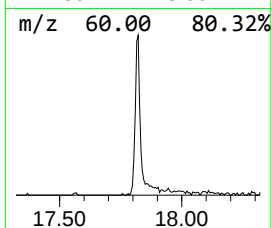
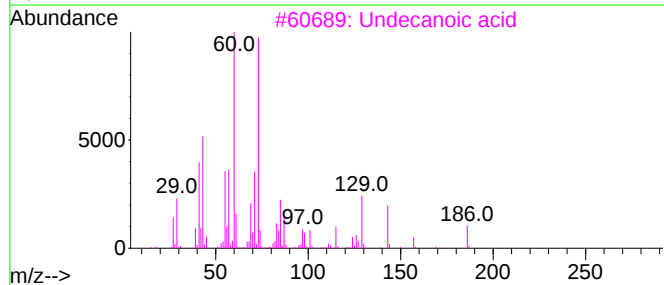
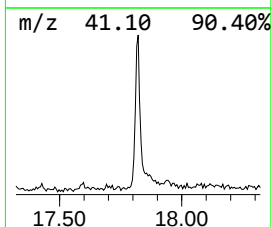
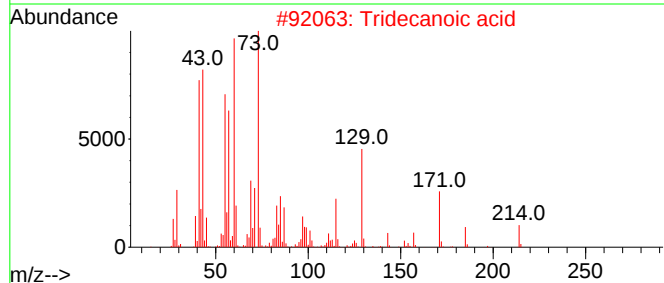
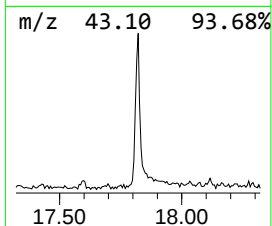
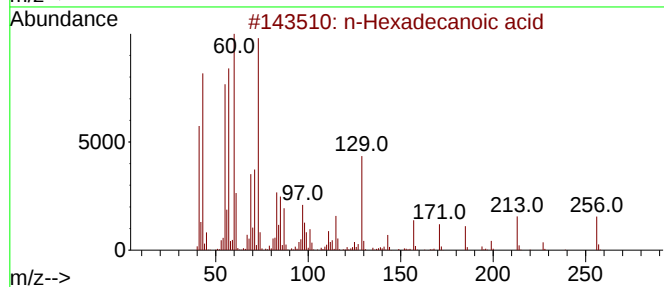
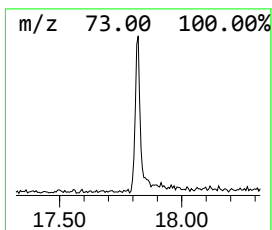
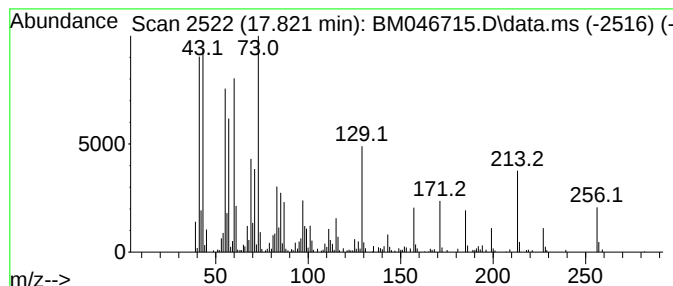
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.821	5.75 ng	369047	Phenanthrene-d10	16.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	86
3			Undecanoic acid	186	C11H22O2	000112-37-8	60
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	60
5			Dodecanoic acid	200	C12H24O2	000143-07-7	58



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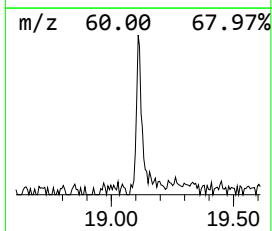
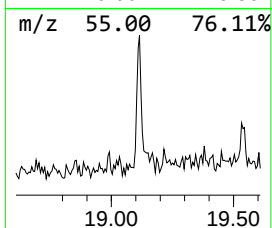
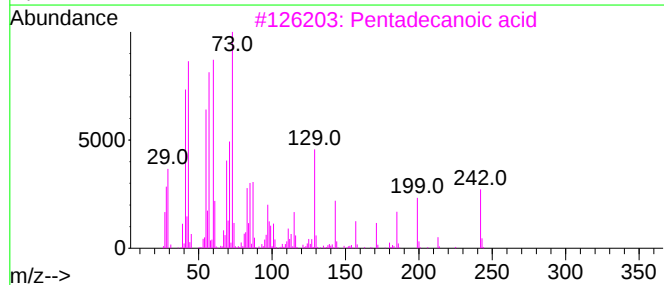
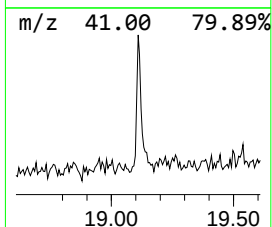
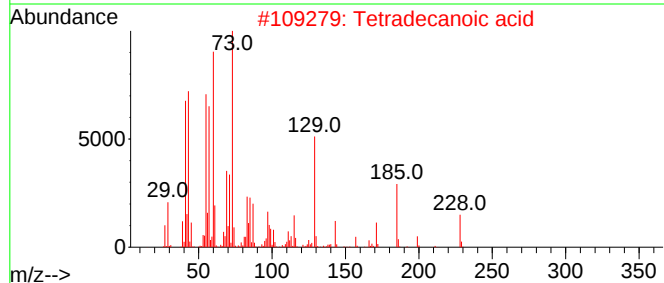
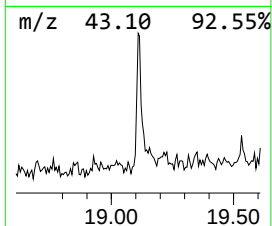
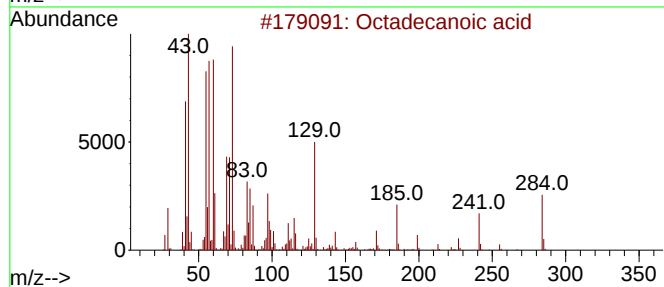
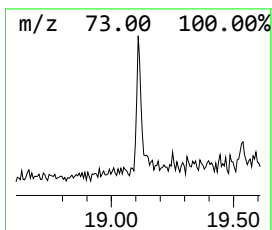
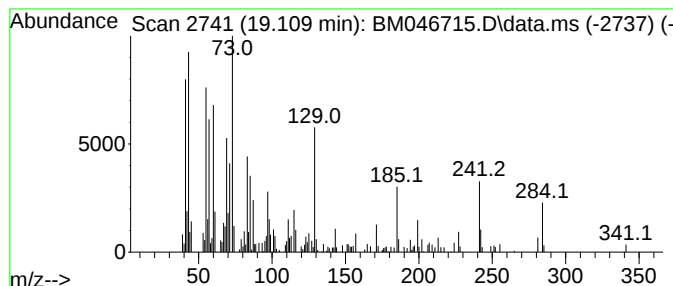
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.110	3.34 ng	164407	Chrysene-d12	21.109

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	95
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4			n-Decanoic acid	172	C10H20O2	000334-48-5	46
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	45



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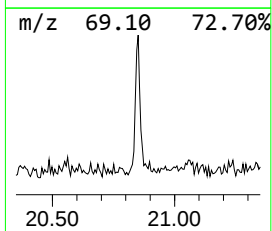
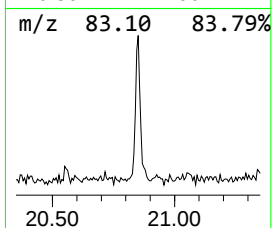
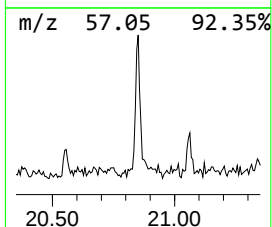
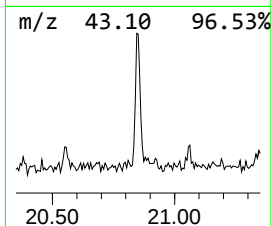
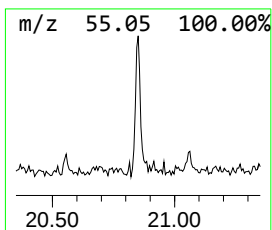
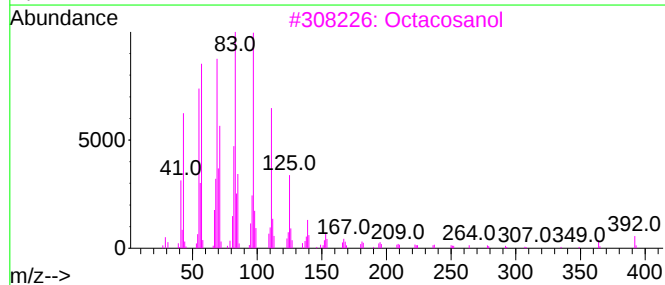
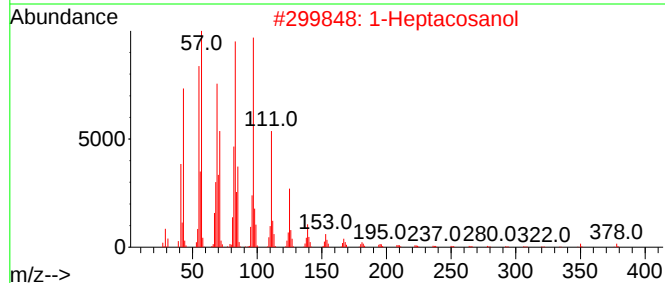
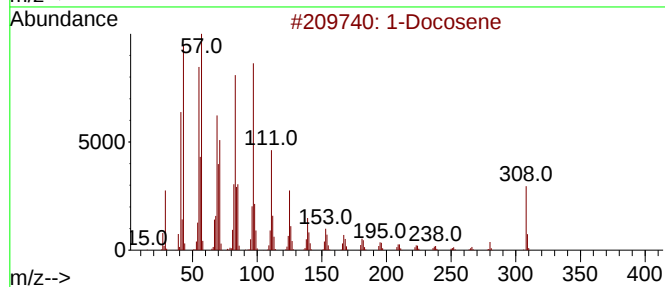
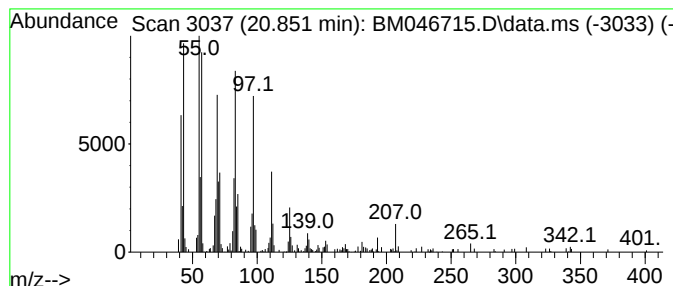
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Docosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.851	4.27 ng	209946	Chrysene-d12	21.109

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	99
2	1-Heptacosanol			396	C27H56O	002004-39-9	93
3	Octacosanol			410	C28H58O	000557-61-9	93
4	n-Tetracosanol-1			354	C24H50O	000506-51-4	93
5	Octacosyl acetate			452	C30H60O2	018206-97-8	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propylene Glycol	3.358	2.5	ng	82366	1	7.487	665772	20.0
(+)-4-Amino-4,...	4.681	3.7	ng	124533	1	7.487	665772	20.0
n-Hexadecanoic ...	17.821	5.8	ng	369047	4	16.886	1282800	20.0
Octadecanoic acid	19.110	3.3	ng	164407	5	21.109	984441	20.0
1-Docosene	20.851	4.3	ng	209946	5	21.109	984441	20.0