

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
 Data File : BM036203.D
 Acq On : 10 Aug 2022 21:49
 Operator : CG/JU
 Sample : N4122-03
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 RBR-200027

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-BM080122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036203.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.528	71	75	81	rBV	109065	139206	1.72%	0.252%
2	5.410	388	395	410	rBV	3277463	4757724	58.67%	8.606%
3	7.028	663	670	685	rBV	3103234	4821145	59.46%	8.721%
4	7.828	795	806	814	rBV	875633	1384221	17.07%	2.504%
5	8.998	997	1005	1013	rBV	1803713	2981313	36.77%	5.393%
6	10.634	1271	1283	1289	rBV	1155537	1925166	23.74%	3.482%
7	12.298	1560	1566	1579	rBV2	74682	139145	1.72%	0.252%
8	13.098	1695	1702	1716	rBV	4115676	5850561	72.15%	10.583%
9	14.363	1909	1917	1927	rBV2	52632	145812	1.80%	0.264%
10	14.469	1927	1935	1942	rVV	1556875	2332667	28.77%	4.220%
11	14.533	1942	1946	1956	rVB	109410	180854	2.23%	0.327%
12	14.869	1998	2003	2012	rBV	91943	152667	1.88%	0.276%
13	15.516	2107	2113	2125	rVB	99917	188002	2.32%	0.340%
14	15.963	2179	2189	2202	rBV	3306388	4695904	57.91%	8.495%
15	16.198	2222	2229	2235	rBV3	62989	117439	1.45%	0.212%
16	17.033	2367	2371	2379	rVB	56203	99930	1.23%	0.181%
17	17.216	2396	2402	2406	rBV	1868188	2623919	32.36%	4.746%
18	17.257	2406	2409	2416	rVV	492313	654056	8.07%	1.183%
19	17.345	2420	2424	2429	rVB	71186	106983	1.32%	0.194%
20	17.886	2512	2516	2521	rBV2	68931	95079	1.17%	0.172%
21	18.115	2547	2555	2564	rBV2	346689	700442	8.64%	1.267%
22	18.286	2579	2584	2588	rBV3	180491	296897	3.66%	0.537%
23	18.592	2632	2636	2640	rVB	75166	98397	1.21%	0.178%
24	18.974	2696	2701	2709	rBV2	665905	1071165	13.21%	1.938%
25	19.062	2712	2716	2720	rVB4	136525	177990	2.20%	0.322%
26	19.268	2746	2751	2758	rBV	995788	1345361	16.59%	2.434%
27	19.633	2804	2813	2822	rBV	740027	1295139	15.97%	2.343%
28	19.839	2842	2848	2853	rBV	6902598	8108791	100.00%	14.668%
29	20.604	2975	2978	2981	rBV	129277	134144	1.65%	0.243%
30	21.109	3060	3064	3071	rBV2	675360	928765	11.45%	1.680%
31	21.392	3106	3112	3116	rBV	2613973	3633867	44.81%	6.573%
32	22.615	3316	3320	3329	rVB	636105	916548	11.30%	1.658%
33	23.739	3505	3511	3518	rBV2	1697613	3182300	39.25%	5.757%

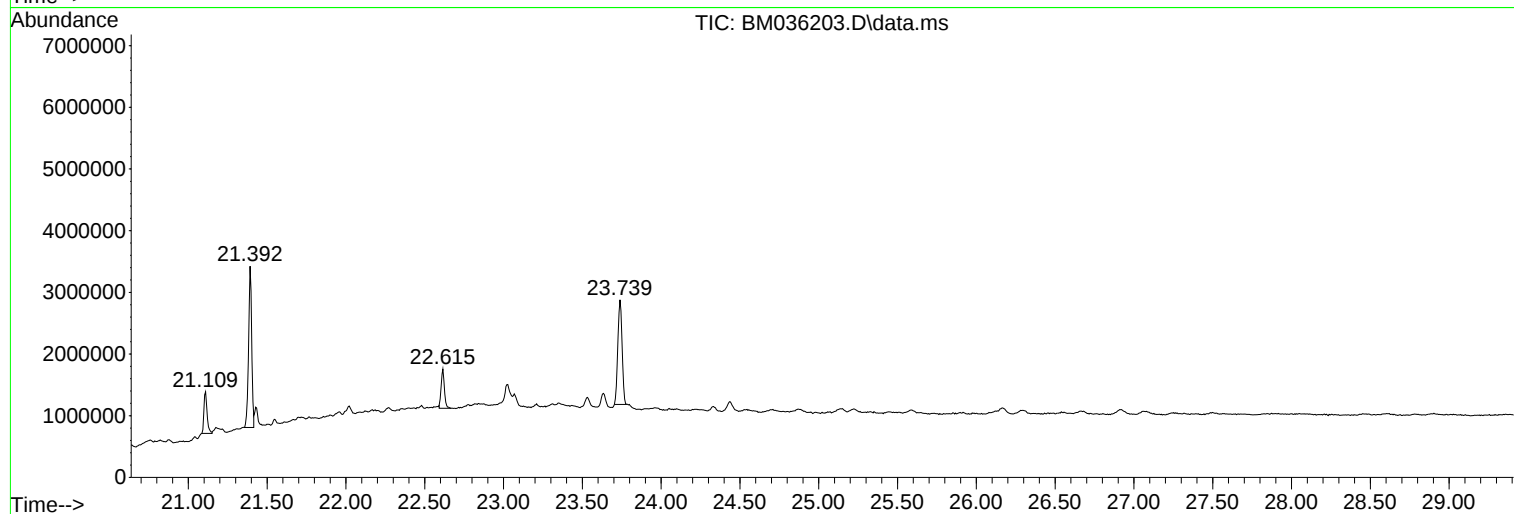
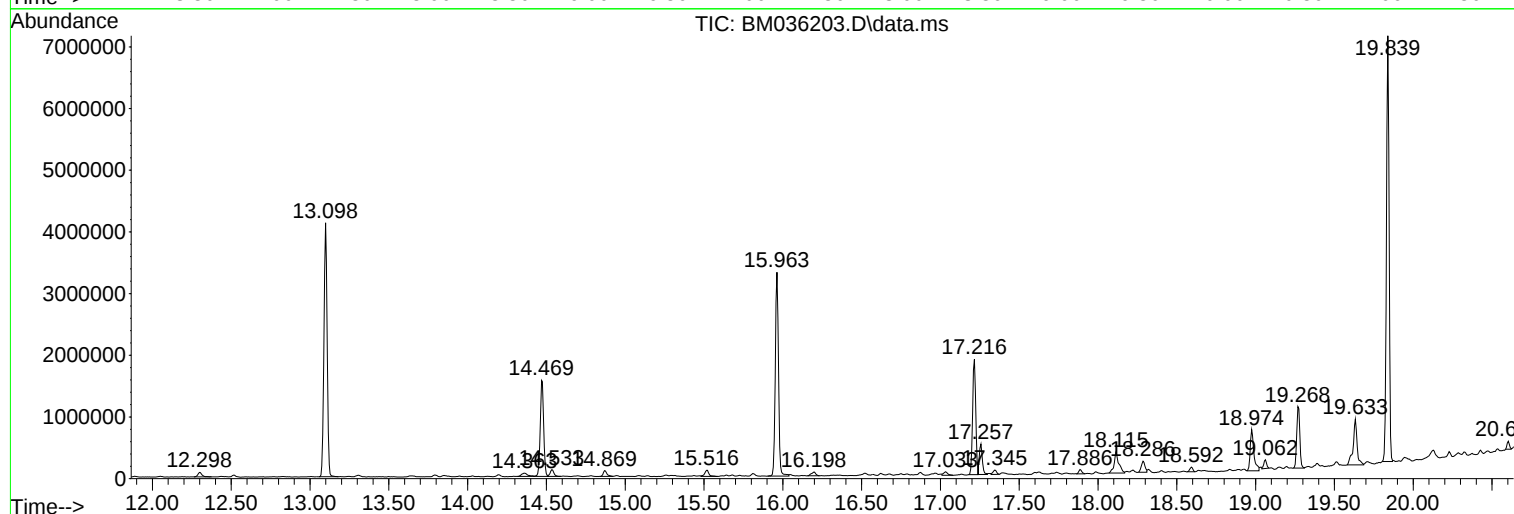
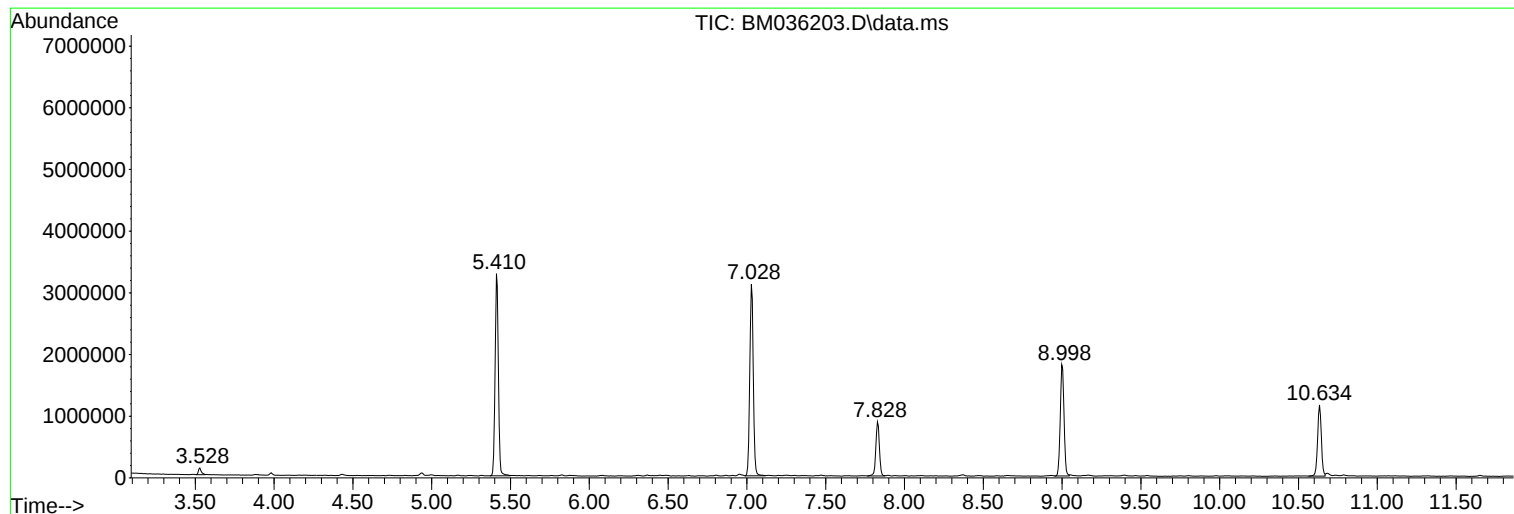
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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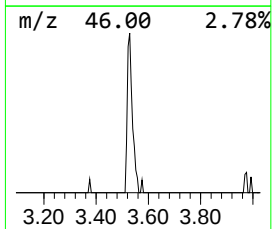
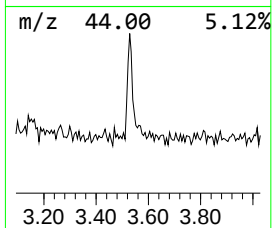
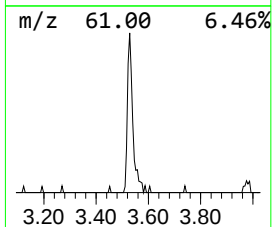
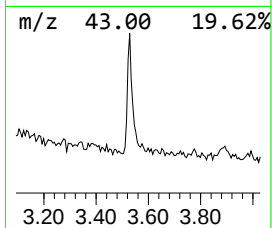
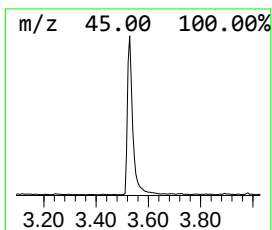
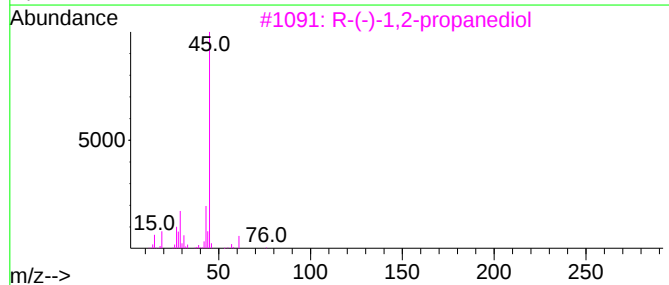
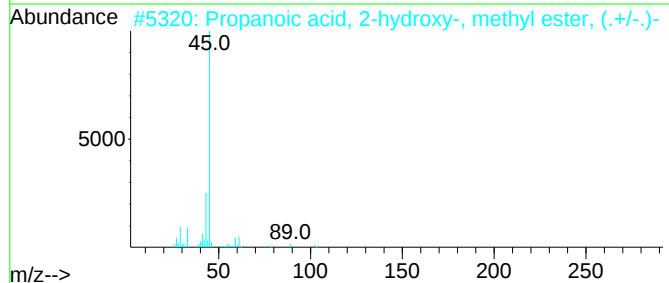
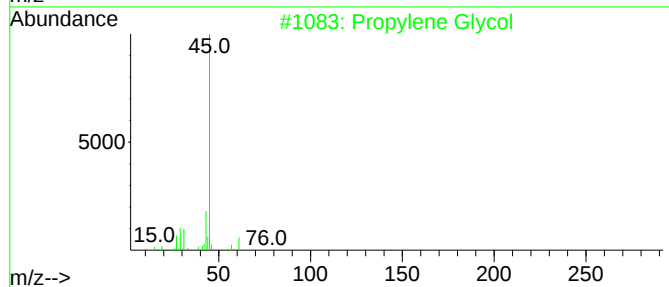
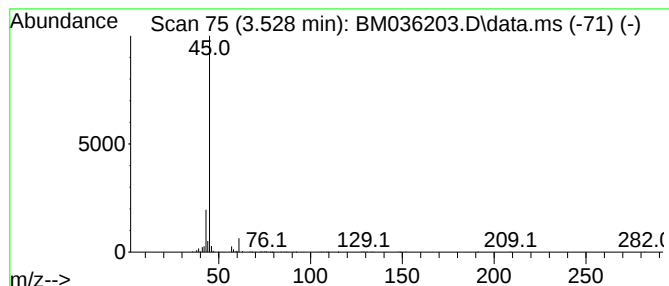
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 Propylene Glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.528	2.01 ng	139206	1,4-Dichlorobenzene-d4	7.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	86
2			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
3			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5			Methyltartronic acid	134	C4H6O5	000595-98-2	9



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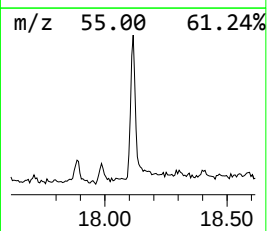
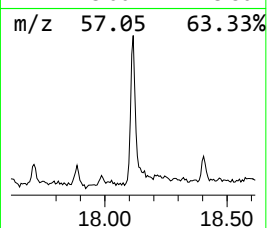
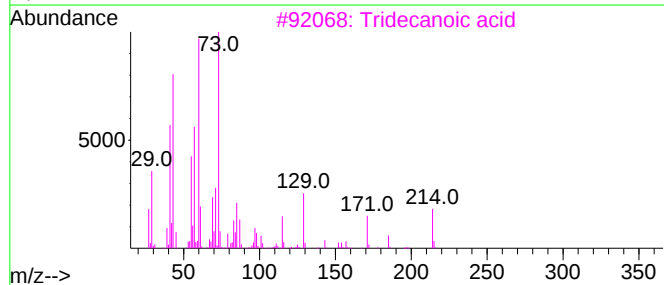
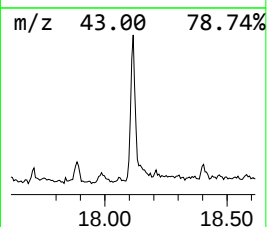
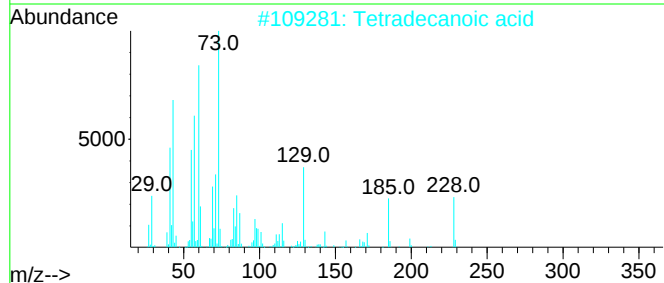
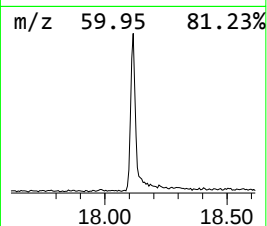
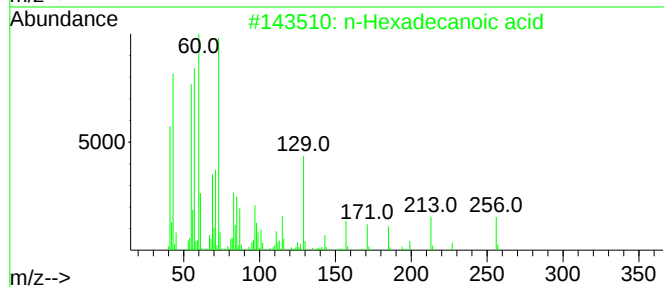
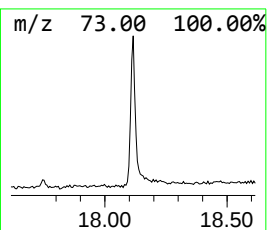
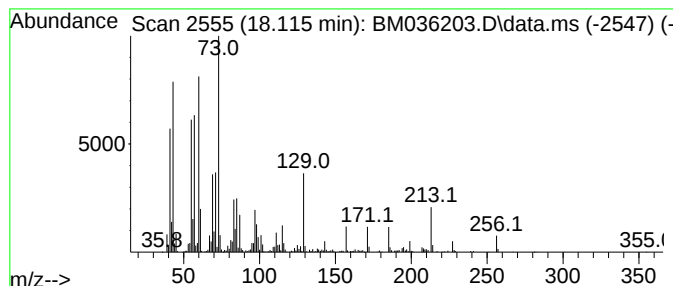
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.116	5.34 ng	700442	Phenanthrene-d10	17.215

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3		Tridecanoic acid	214	C13H26O2	000638-53-9	89
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5		Dodecanoic acid	200	C12H24O2	000143-07-7	64



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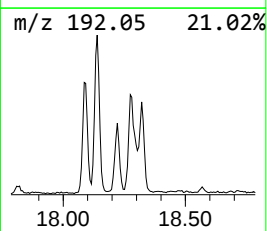
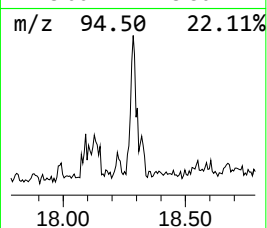
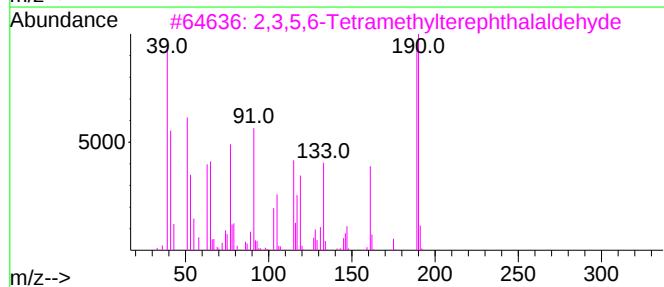
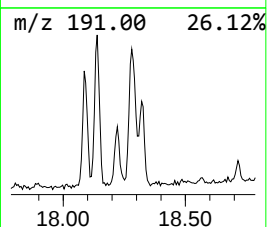
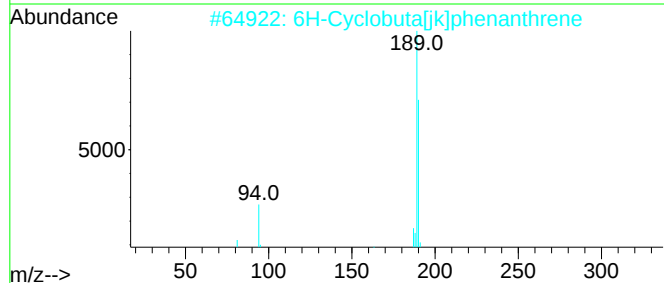
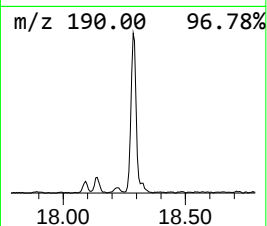
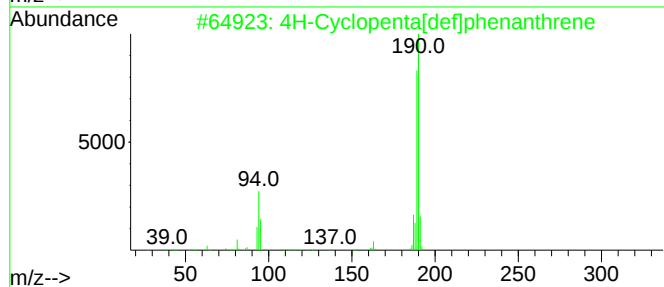
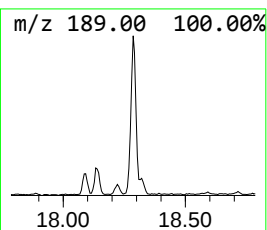
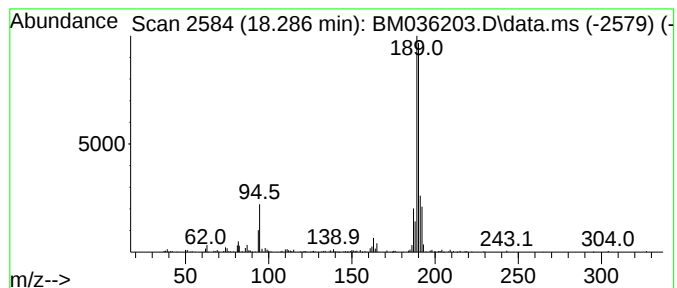
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Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.286	2.26 ng	296897	Phenanthrene-d10	17.215

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	72
3			2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
4			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
5			L-Ethionine, 2TMS derivative	307	C12H29NO2SSi2	055255-82-8	23



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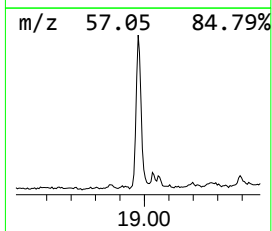
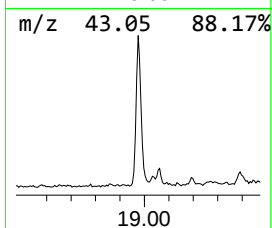
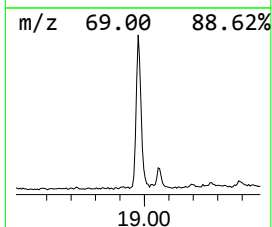
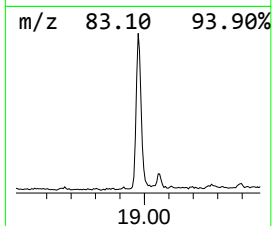
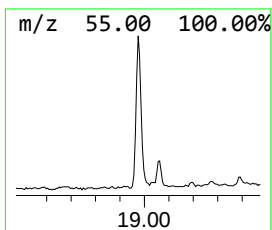
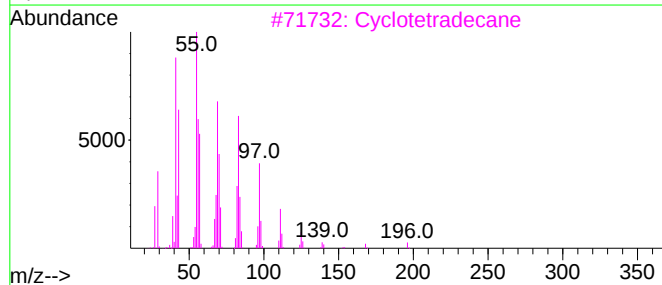
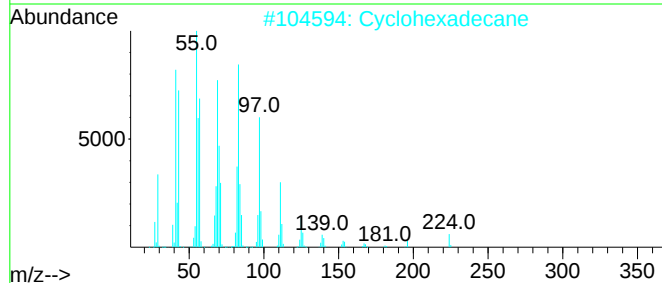
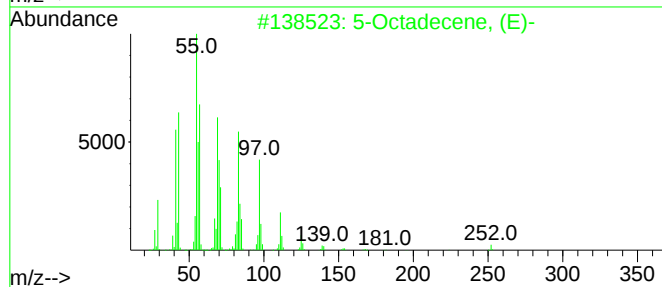
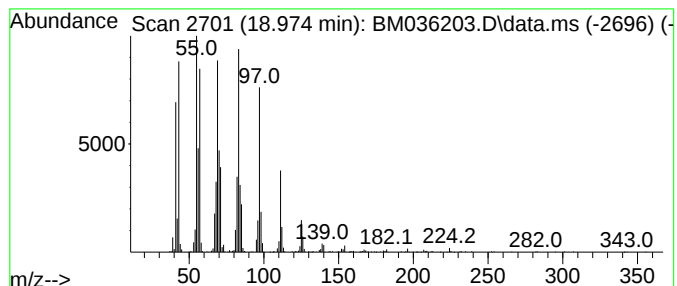
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Peak Number 4 5-Octadecene, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.974	8.16 ng	1071170	Phenanthrene-d10	17.215

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Octadecene, (E)-	252	C18H36	007206-21-5	99
2			Cyclohexadecane	224	C16H32	000295-65-8	98
3			Cyclotetradecane	196	C14H28	000295-17-0	97
4			1-Octadecanol	270	C18H38O	000112-92-5	94
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	94



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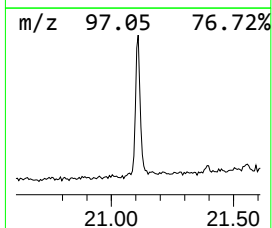
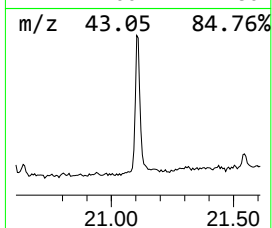
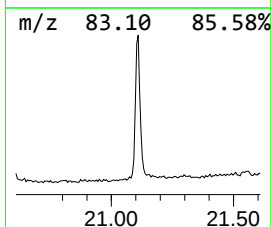
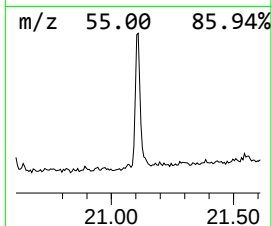
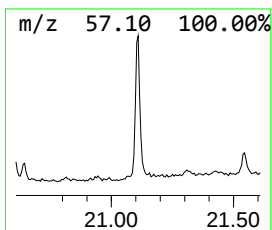
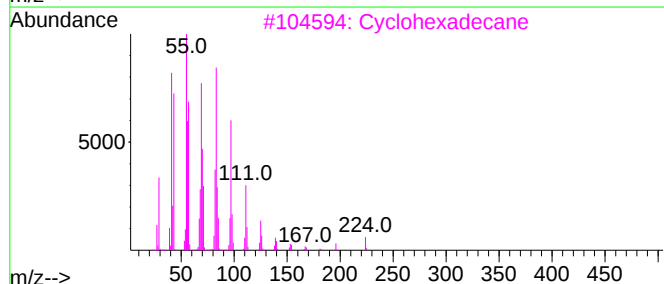
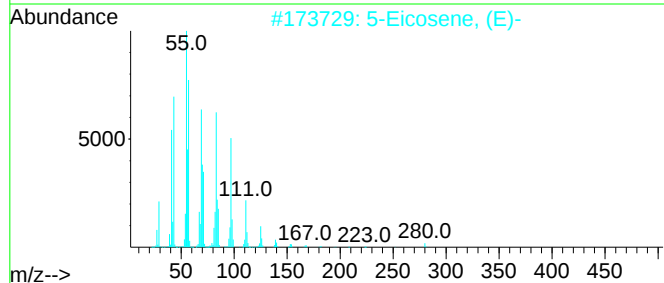
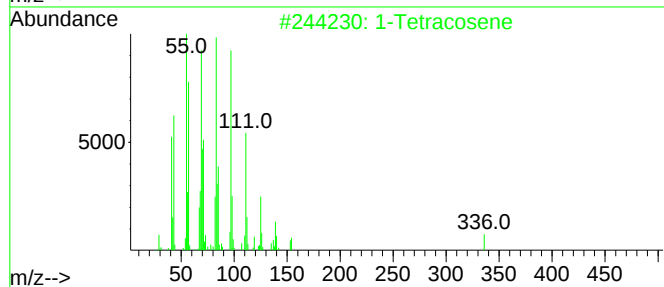
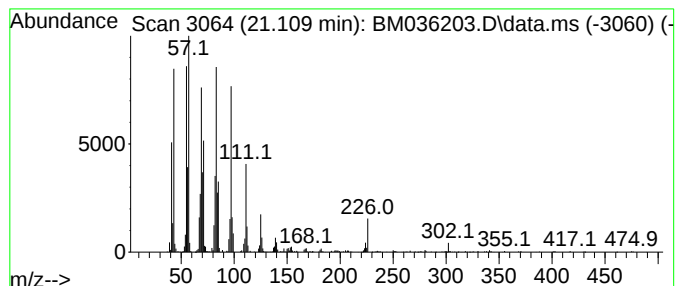
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Peak Number 5 1-Tetracosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.109	5.11 ng	928765	Chrysene-d12	21.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tetracosene	336	C24H48	010192-32-2	99
2			5-Eicosene, (E)-	280	C20H40	074685-30-6	98
3			Cyclohexadecane	224	C16H32	000295-65-8	94
4			Cyclotetracosane	336	C24H48	000297-03-0	94
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	94



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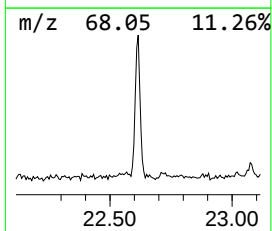
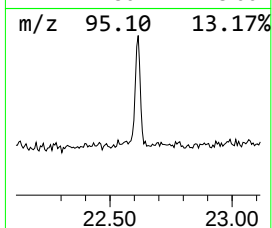
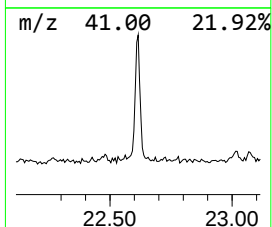
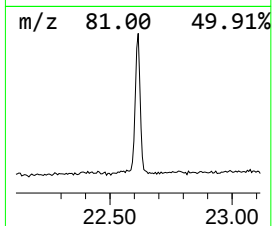
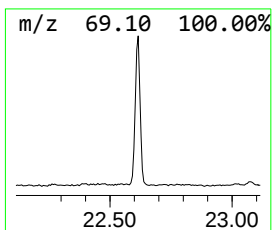
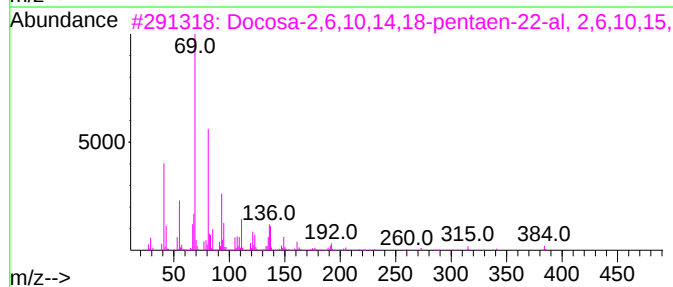
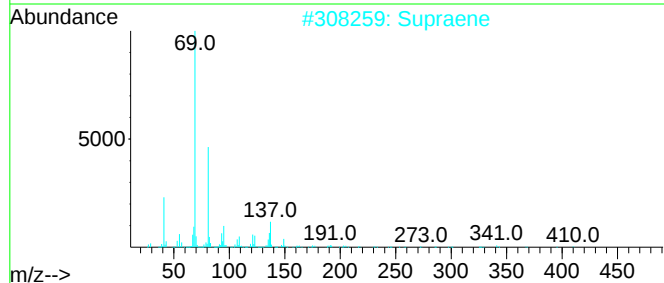
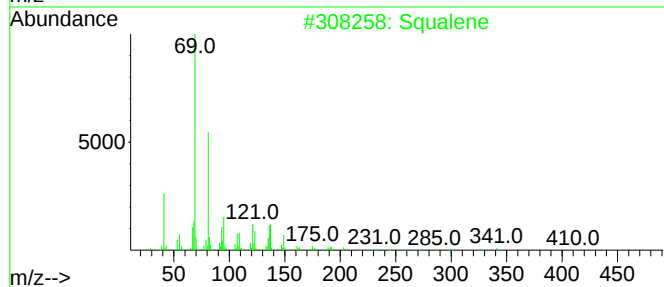
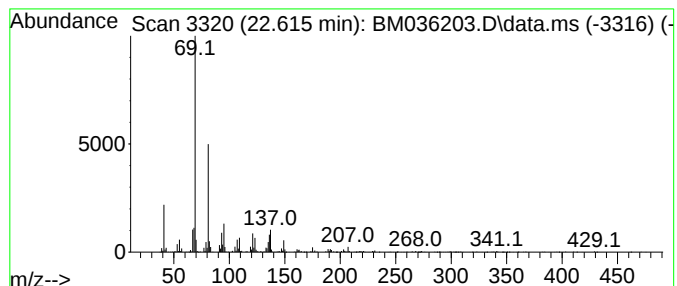
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.615	5.76 ng	916548	Perylene-d12	23.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	94
2			Supraene	410	C30H50	007683-64-9	91
3			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	87
5			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036203.D
Acq On : 10 Aug 2022 21:49
Operator : CG/JU
Sample : N4122-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RBR-200027

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propylene Glycol	3.528	2.0	ng	139206	1	7.828	1384220	20.0
n-Hexadecanoic ...	18.116	5.3	ng	700442	4	17.215	2623920	20.0
4H-Cyclopenta[d...]	18.286	2.3	ng	296897	4	17.215	2623920	20.0
5-Octadecene, (E)-	18.974	8.2	ng	1071170	4	17.215	2623920	20.0
1-Tetracosene	21.109	5.1	ng	928765	5	21.392	3633870	20.0
Squalene	22.615	5.8	ng	916548	6	23.739	3182300	20.0