

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
 Data File : BG058566.D
 Acq On : 1 Aug 2023 17:23
 Operator : MA/JU
 Sample : 03715-05
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 T842-FH-03-CT

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_G\Methods\8270-BG072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058566.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.383	384	390	402	rBV	280465	462860	13.27%	2.608%
2	6.987	653	663	677	rBV	400900	704580	20.20%	3.970%
3	7.815	795	804	812	rBV	196774	335551	9.62%	1.890%
4	8.979	992	1002	1012	rBV	198630	373314	10.70%	2.103%
5	10.612	1274	1280	1294	rBV	276220	506867	14.53%	2.856%
6	13.080	1693	1700	1715	rBV	757651	1191436	34.16%	6.712%
7	14.108	1870	1875	1884	rBV8	15731	48774	1.40%	0.275%
8	14.460	1929	1935	1944	rVB	458704	715493	20.52%	4.031%
9	15.824	2157	2167	2180	rBV	2269773	3487648	100.00%	19.649%
10	15.959	2184	2190	2210	rVB	668974	1055653	30.27%	5.947%
11	17.046	2371	2375	2381	rVB	35458	46393	1.33%	0.261%
12	17.210	2396	2403	2409	rBV	550037	844085	24.20%	4.756%
13	18.097	2549	2554	2564	rBV	237276	362513	10.39%	2.042%
14	18.297	2583	2588	2593	rBV4	18073	40306	1.16%	0.227%
15	19.261	2743	2752	2757	rBV10	23501	74887	2.15%	0.422%
16	19.372	2765	2771	2785	rVB3	115150	203776	5.84%	1.148%
17	19.719	2824	2830	2831	rBV6	25563	36848	1.06%	0.208%
18	19.825	2842	2848	2855	rVB	1494978	1933448	55.44%	10.893%
19	20.512	2961	2965	2971	rBV2	39314	50171	1.44%	0.283%
20	21.446	3118	3124	3140	rBV2	568253	899608	25.79%	5.068%
21	22.557	3309	3313	3319	rVB4	26887	49444	1.42%	0.279%
22	22.851	3358	3363	3369	rVB6	28233	63298	1.81%	0.357%
23	23.033	3388	3394	3404	rVB	95441	189691	5.44%	1.069%
24	24.519	3637	3647	3662	rVB	363149	1023164	29.34%	5.764%
25	25.148	3744	3754	3765	rBV2	435677	1232445	35.34%	6.944%
26	31.117	4752	4770	4790	rBV5	329156	1817302	52.11%	10.239%

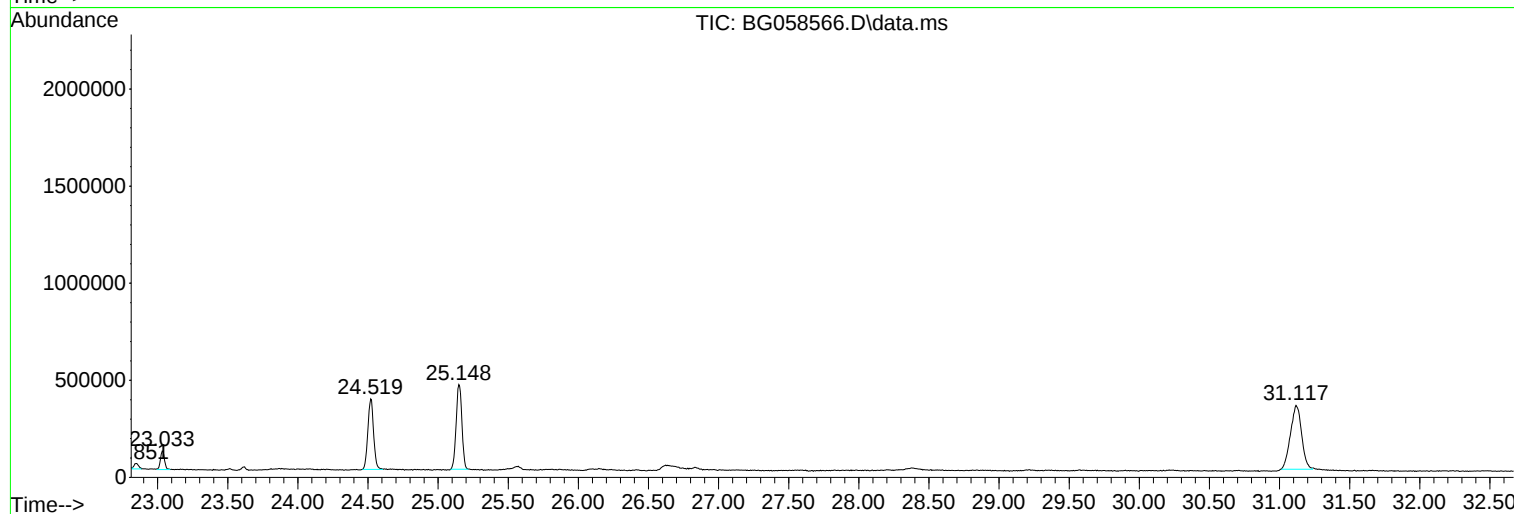
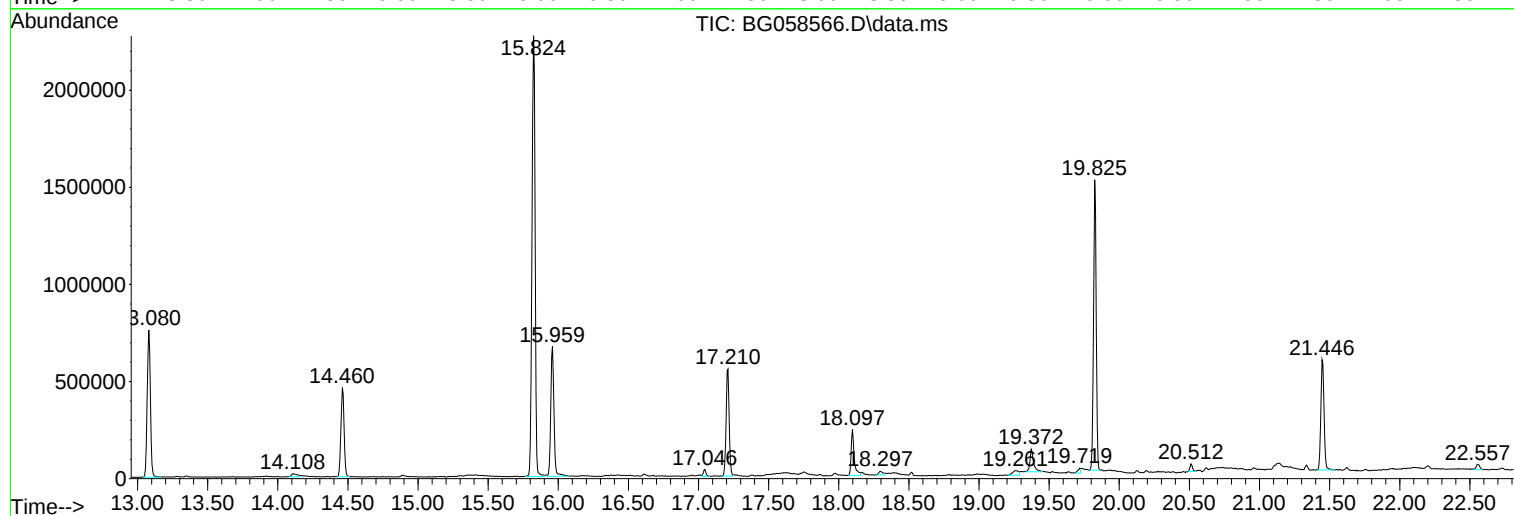
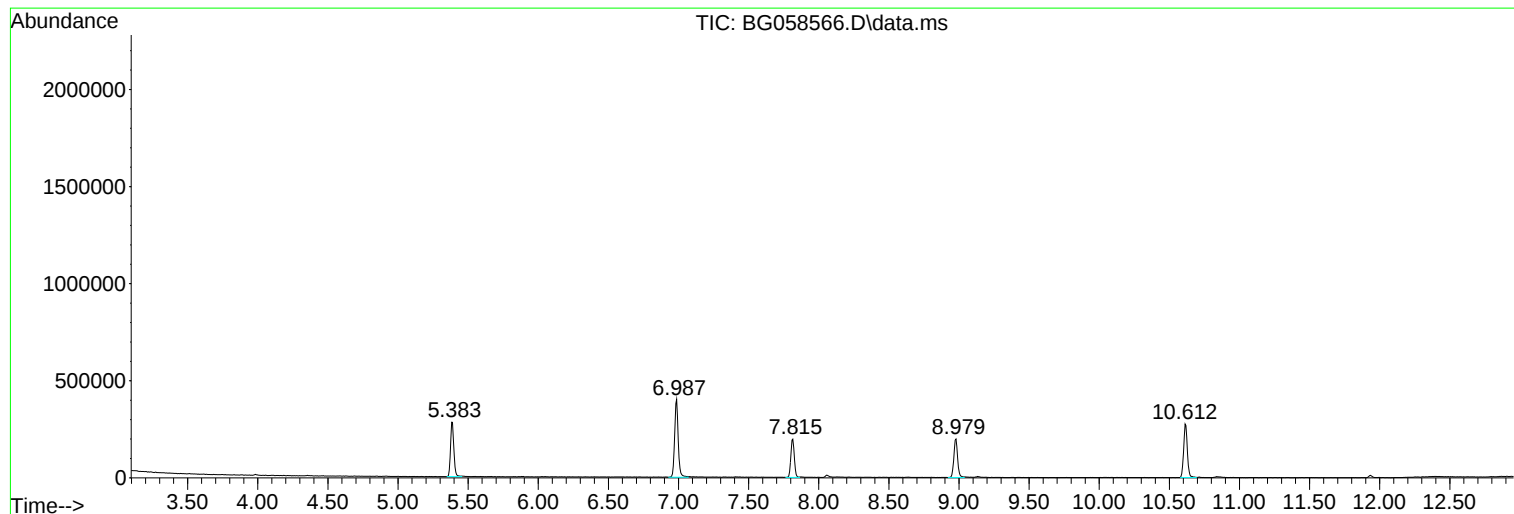
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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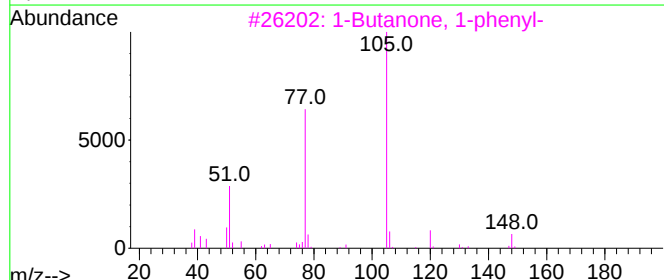
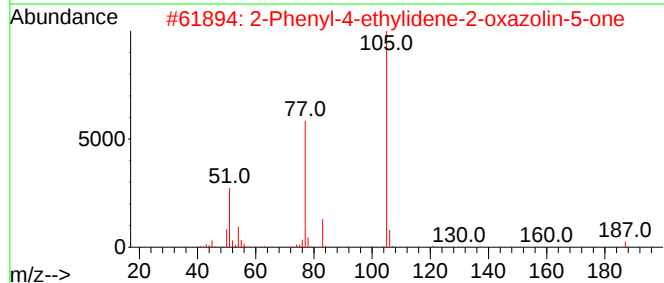
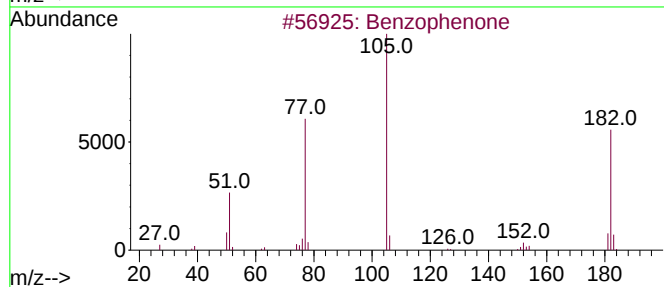
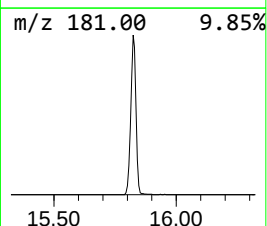
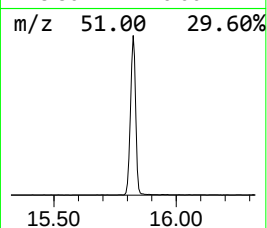
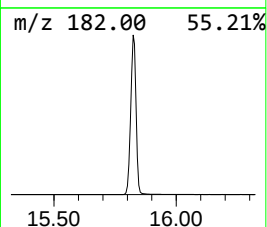
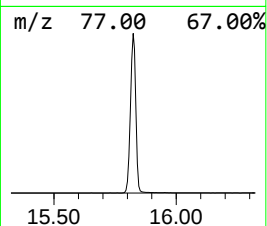
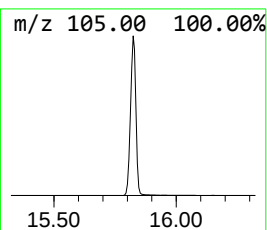
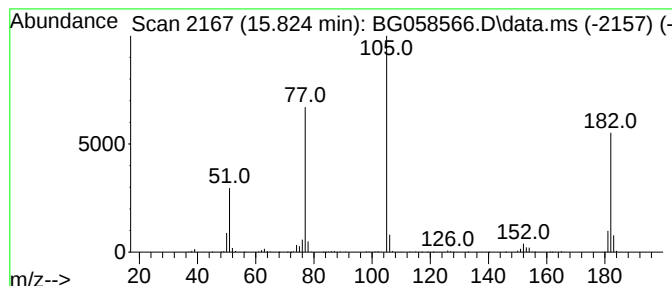
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.823	97.49 ng	3487650	Acenaphthene-d10	14.460

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	47
3			1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	47
4			Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	47
5			Vinyl benzoate	148	C9H8O2	000769-78-8	47



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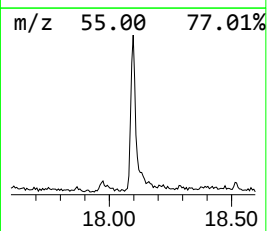
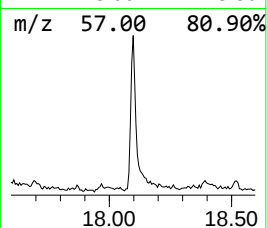
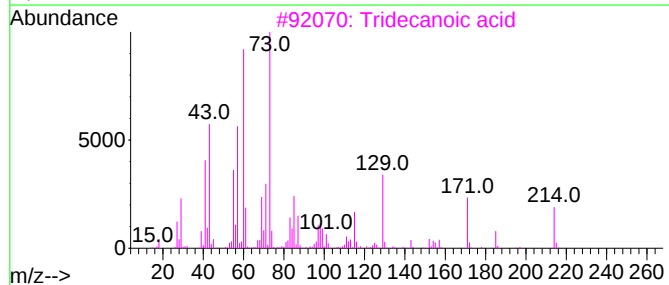
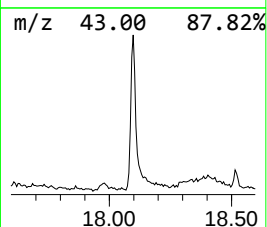
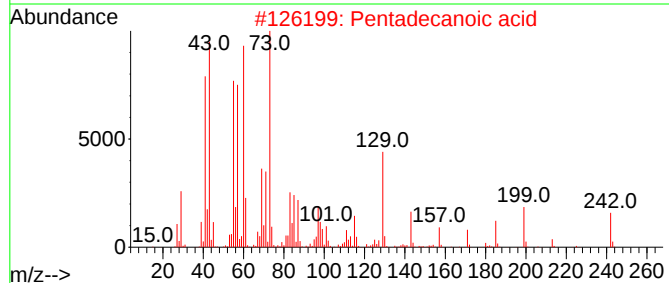
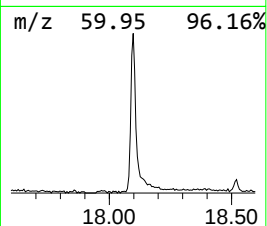
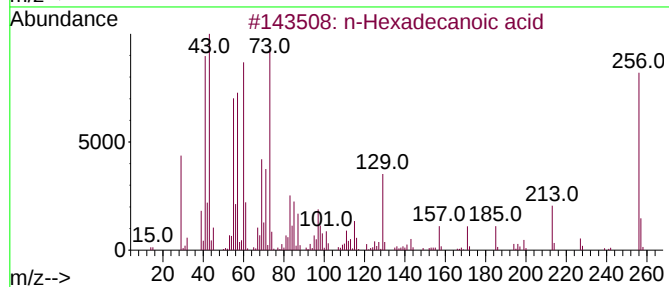
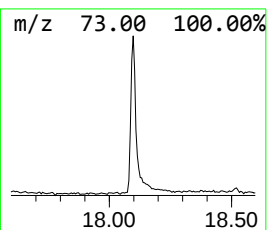
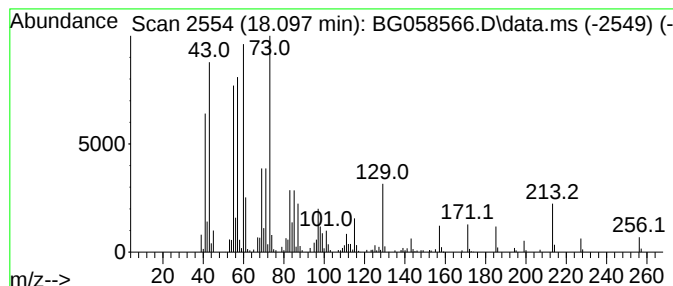
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.097	8.59 ng	362513	Phenanthrene-d10	17.210

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



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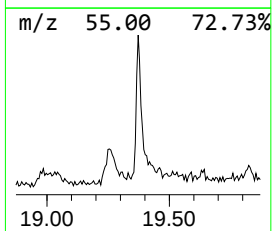
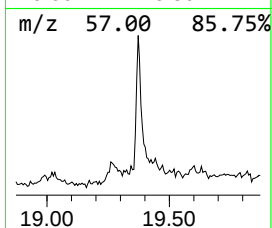
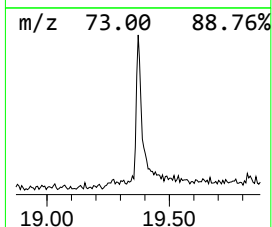
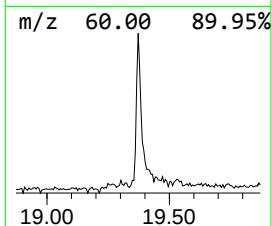
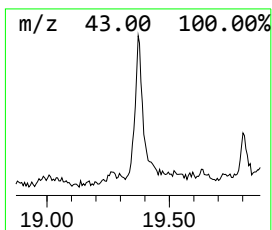
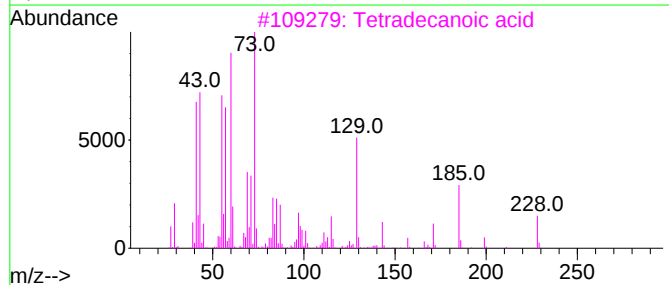
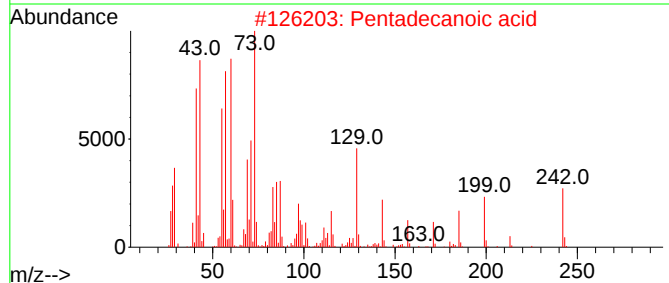
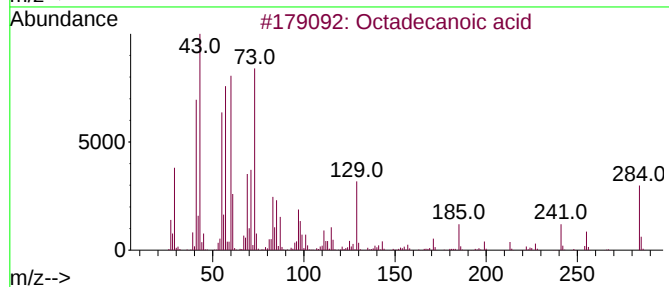
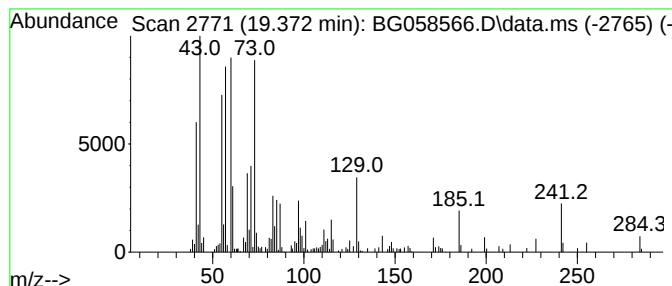
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.372	4.53 ng	203776	Chrysene-d12	21.446

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	95
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72



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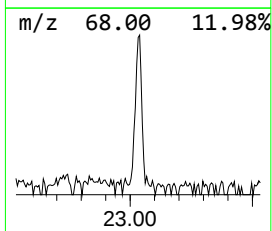
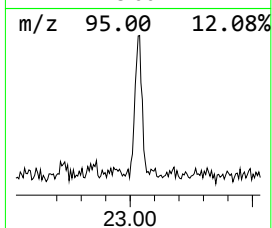
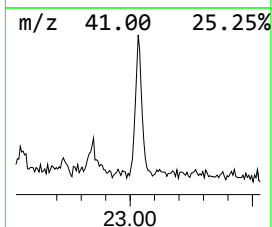
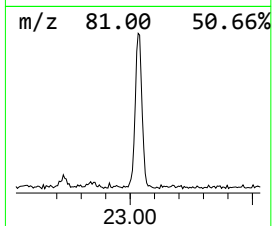
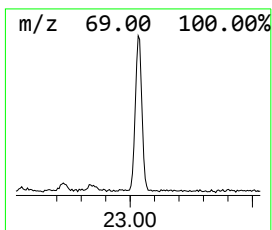
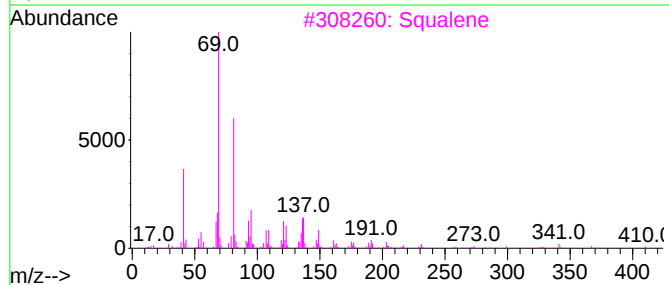
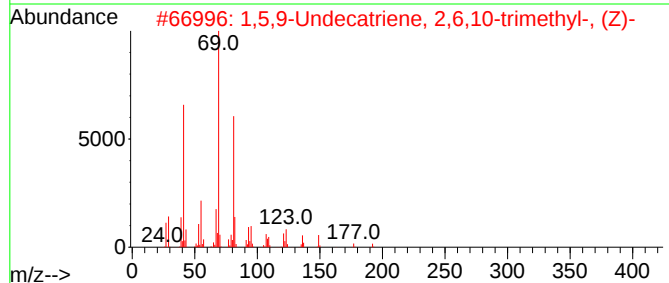
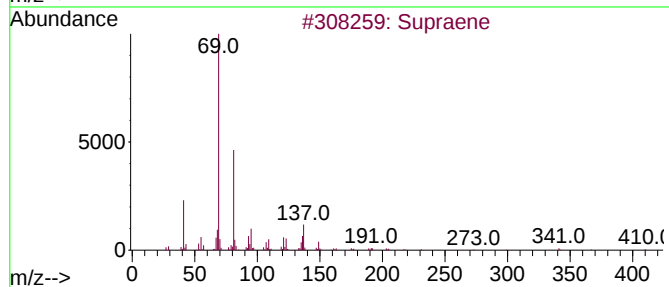
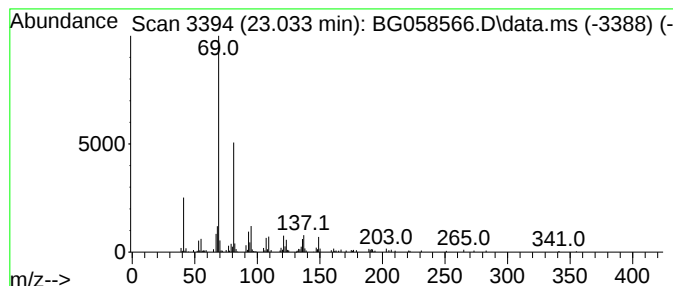
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Peak Number 4 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.033	3.71 ng	189691	Perylene-d12	24.519

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	87
2			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	86
3			Squalene	410	C30H50	000111-02-4	86
4			trans-Farnesol	222	C15H26O	000106-28-5	80
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	78



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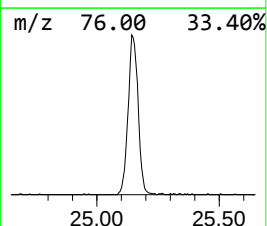
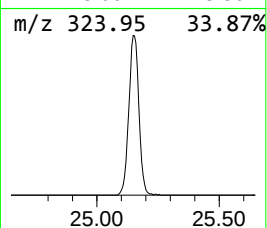
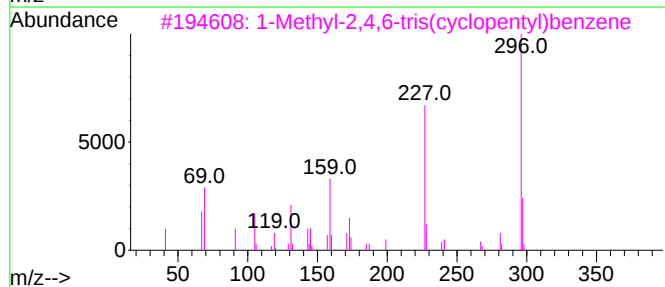
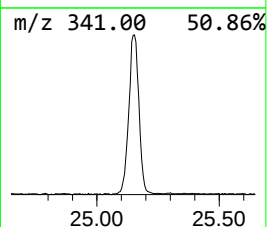
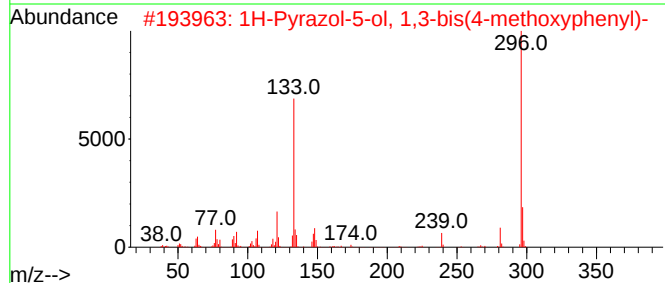
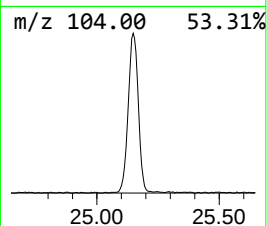
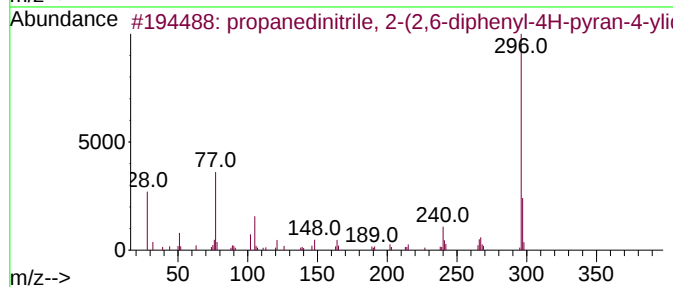
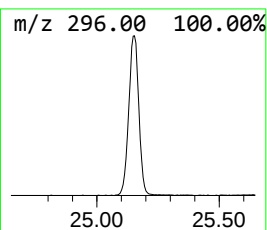
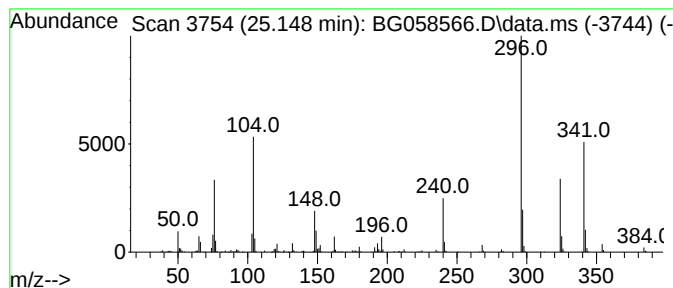
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Peak Number 5 unknown25.148 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.148	24.09 ng	1232450	Perylene-d12	24.519

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			propanedinitrile, 2-(2,6-dipheny...	296	C20H12N2O	1000402-09-2	27
2			1H-Pyrazol-5-ol, 1,3-bis(4-metho...	296	C17H16N2O3	1000337-80-1	22
3			1-Methyl-2,4,6-tris(cyclopentyl)...	296	C22H32	100325-74-4	22
4			trans-4'-Dimethylamino-3-nitroch...	296	C17H16N2O3	1000234-56-7	16
5			Phthalic anhydride	148	C8H4O3	000085-44-9	14



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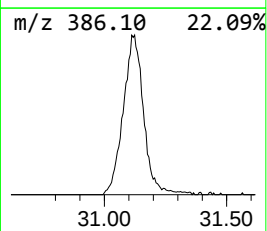
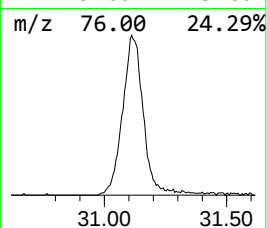
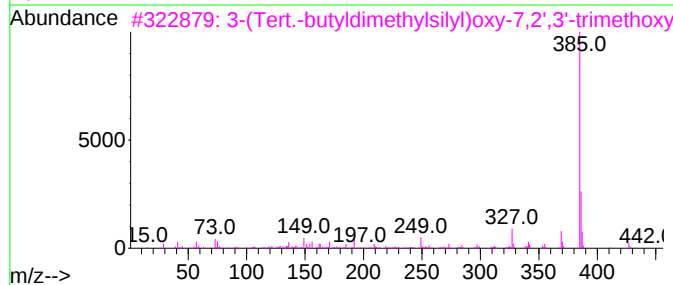
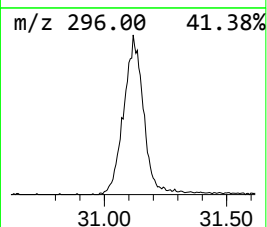
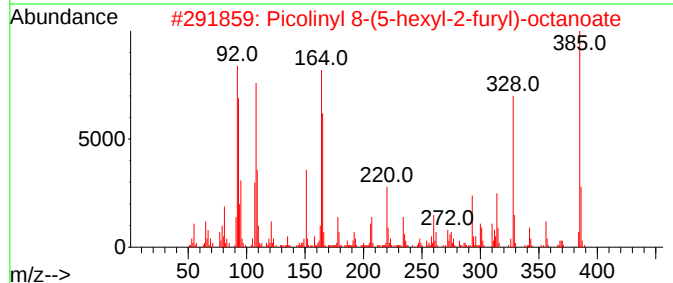
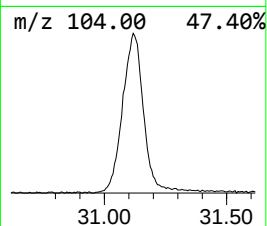
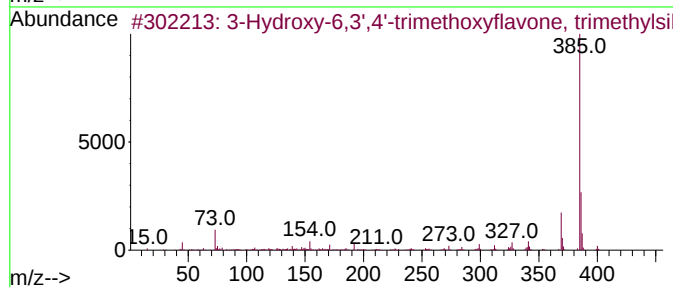
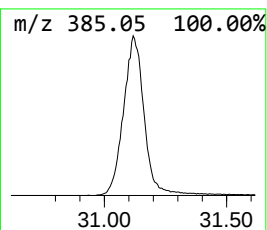
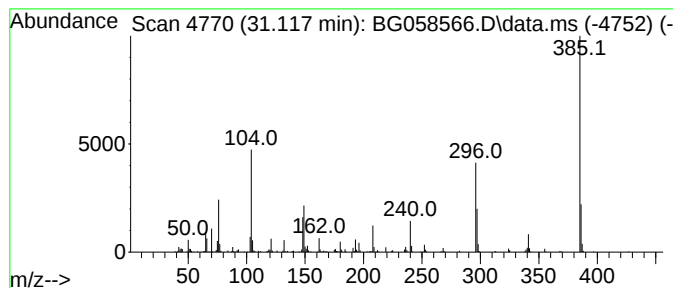
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown31.117 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.117	35.52 ng	1817300	Perylene-d12	24.519

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hydroxy-6,3',4'-trimethoxyflav...	400	C21H24O6Si	1000448-94-7	22
2			Picolinyl 8-(5-hexyl-2-furyl)-oc...	385	C24H35NO3	1000335-93-0	22
3			3-(Tert.-butyldimethylsilyl)oxy-...	442	C24H30O6Si	1000454-35-9	12
4			3-(Tert.-butyldimethylsilyl)oxy-...	442	C24H30O6Si	1000454-18-6	12
5			3-(4-Methylphenyl)-4-oxo-2-thiox...	400	C20H24N2O5S2Si	1000512-11-8	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058566.D
Acq On : 1 Aug 2023 17:23
Operator : MA/JU
Sample : 03715-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
T842-FH-03-CT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.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
Benzophenone	15.823	97.5	ng	3487650	3	14.460	715493	20.0
n-Hexadecanoic ...	18.097	8.6	ng	362513	4	17.210	844085	20.0
Octadecanoic acid	19.372	4.5	ng	203776	5	21.446	899608	20.0
Supraene	23.033	3.7	ng	189691	6	24.519	1023160	20.0
unknown25.148	25.148	24.1	ng	1232450	6	24.519	1023160	20.0
unknown31.117	31.117	35.5	ng	1817300	6	24.519	1023160	20.0