

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
 Data File : BG058567.D
 Acq On : 1 Aug 2023 18:03
 Operator : MA/JU
 Sample : 03715-06
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

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

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: BG058567.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.912	305	310	318	rVB	40755	62669	1.56%	0.214%
2	5.388	385	391	401	rBV	951323	1477890	36.88%	5.041%
3	6.992	653	664	683	rBV	898780	1587836	39.62%	5.416%
4	7.815	795	804	810	rBV	193430	331014	8.26%	1.129%
5	8.978	993	1002	1018	rBV	547881	991411	24.74%	3.382%
6	10.617	1273	1281	1295	rBV	271873	498157	12.43%	1.699%
7	13.079	1693	1700	1712	rBV	1441277	2285760	57.04%	7.797%
8	14.107	1868	1875	1895	rBV3	26192	103310	2.58%	0.352%
9	14.460	1929	1935	1946	rVB	443568	710712	17.74%	2.424%
10	14.883	2001	2007	2020	rBV3	19902	40286	1.01%	0.137%
11	15.823	2160	2167	2181	rBV	2484601	4007397	100.00%	13.670%
12	15.958	2183	2190	2199	rBV	1212569	1842860	45.99%	6.286%
13	16.404	2259	2266	2276	rVB	35804	67595	1.69%	0.231%
14	17.209	2396	2403	2410	rBV	544243	849806	21.21%	2.899%
15	18.102	2549	2555	2573	rBV	874618	1367062	34.11%	4.663%
16	19.231	2743	2747	2748	rBV	56479	67110	1.67%	0.229%
17	19.254	2748	2751	2764	rVV	105933	201129	5.02%	0.686%
18	19.377	2767	2772	2788	rBV	685541	1017415	25.39%	3.471%
19	19.736	2825	2833	2843	rBV5	32315	142958	3.57%	0.488%
20	19.830	2843	2849	2864	rVB	2512038	3406383	85.00%	11.620%
21	20.506	2958	2964	2968	rBV5	23433	49883	1.24%	0.170%
22	20.617	2979	2983	2987	rBV2	46087	65168	1.63%	0.222%
23	21.128	3062	3070	3087	rBV5	72897	314343	7.84%	1.072%
24	21.446	3118	3124	3133	rBV	532050	858432	21.42%	2.928%
25	21.622	3151	3154	3158	rVB2	35707	46682	1.16%	0.159%
26	22.198	3249	3252	3257	rVB2	41680	59112	1.48%	0.202%
27	22.674	3328	3333	3341	rBV3	19368	41534	1.04%	0.142%
28	22.844	3356	3362	3373	rBV5	92603	256062	6.39%	0.873%
29	23.032	3388	3394	3401	rBV	203926	410031	10.23%	1.399%
30	23.285	3432	3437	3444	rVB2	37647	77765	1.94%	0.265%
31	23.502	3469	3474	3480	rVB2	29806	55492	1.38%	0.189%
32	23.614	3487	3493	3499	rVB3	38148	75909	1.89%	0.259%
33	24.518	3637	3647	3660	rBV	365769	1028645	25.67%	3.509%
34	25.153	3744	3755	3769	rVB	704680	2023637	50.50%	6.903%
35	31.128	4752	4772	4792	rBV3	511882	2894195	72.22%	9.873%

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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

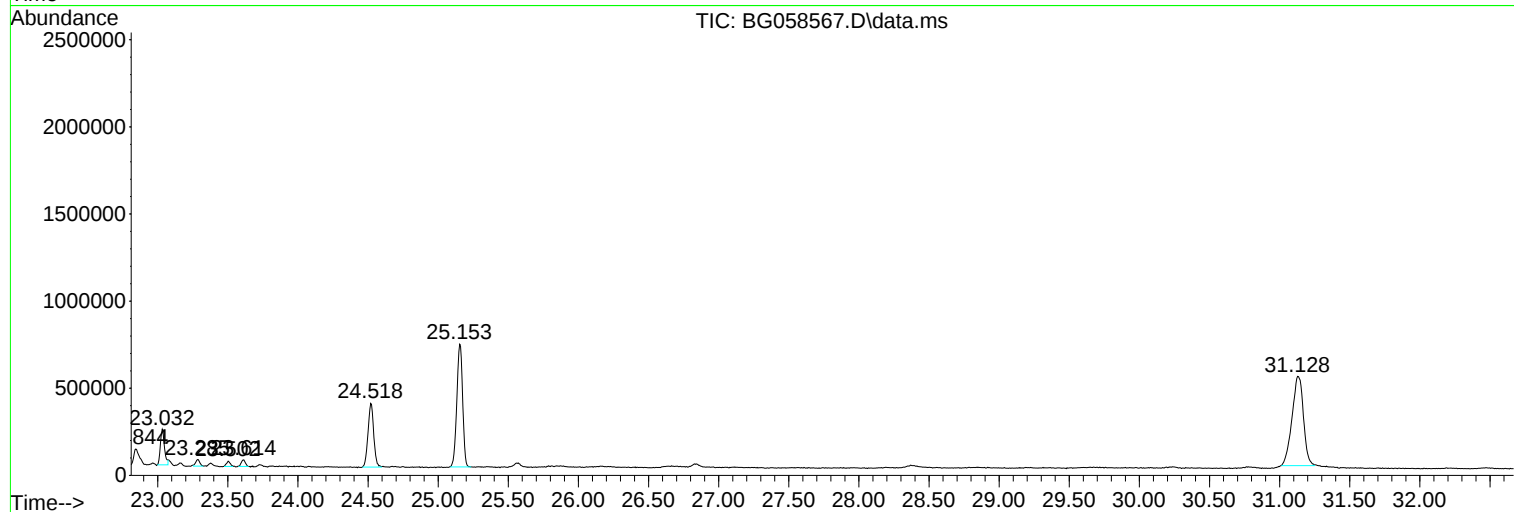
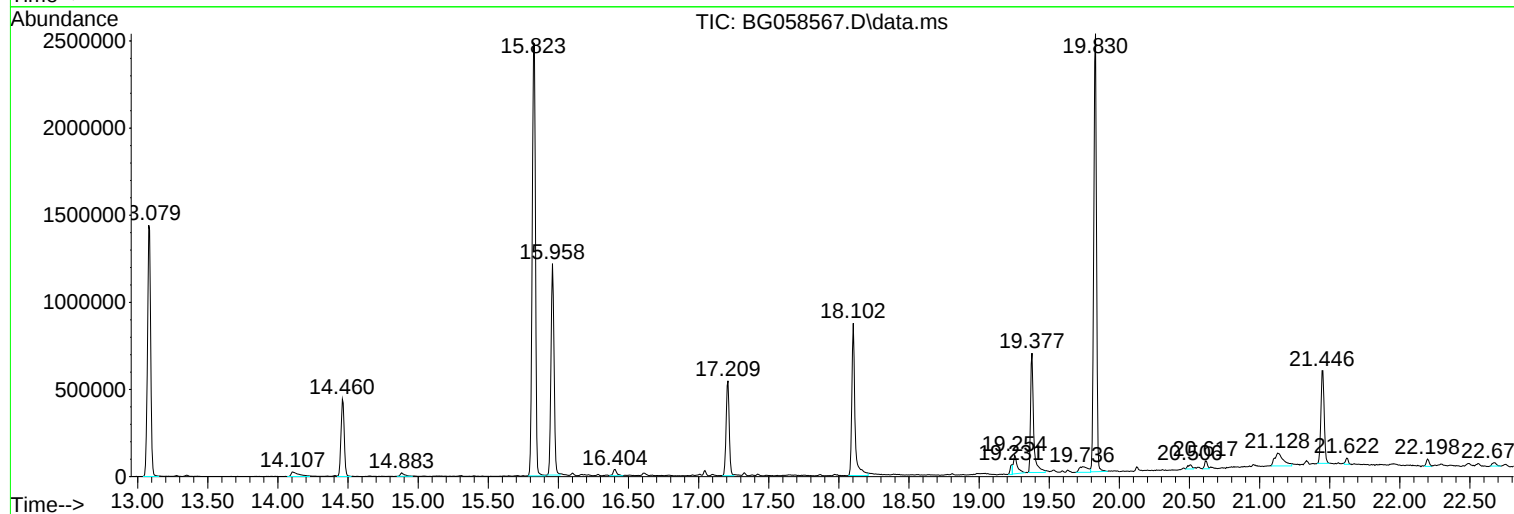
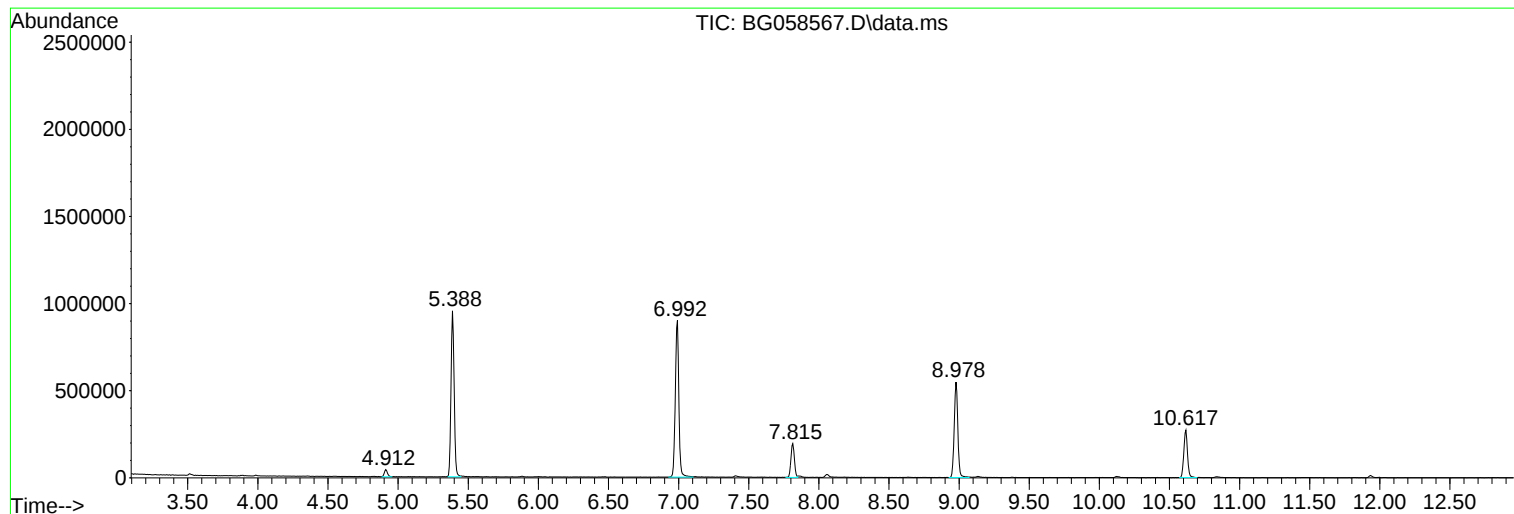
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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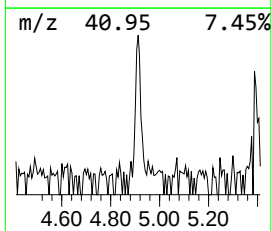
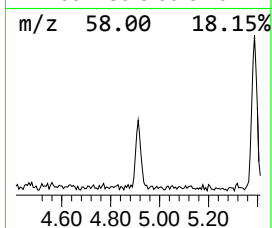
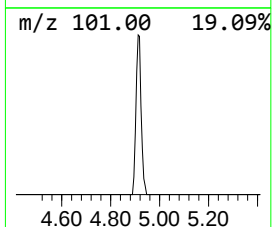
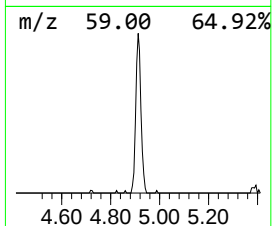
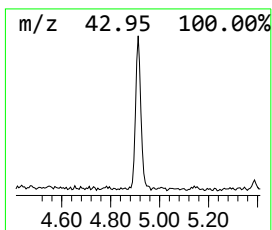
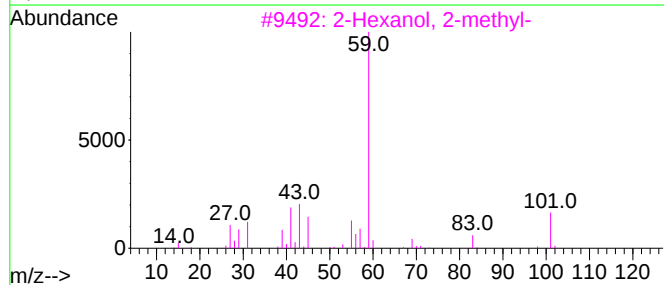
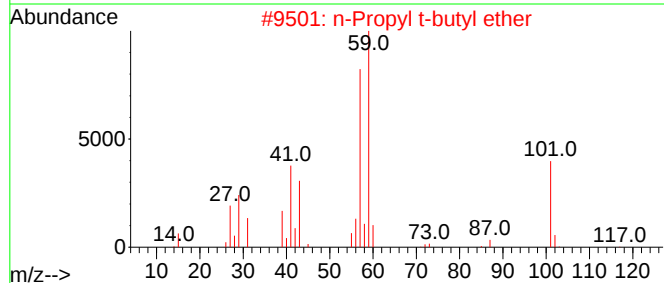
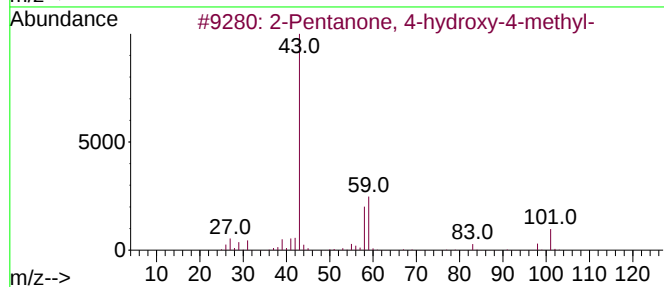
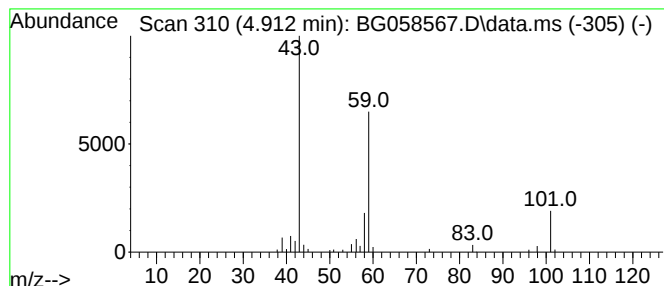
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.912	3.79 ng	62669	1,4-Dichlorobenzene-d4	7.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53		
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25		
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		



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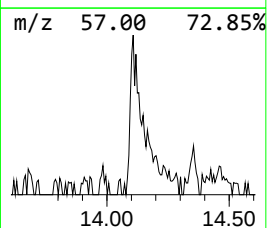
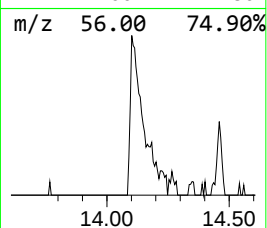
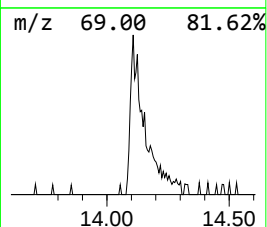
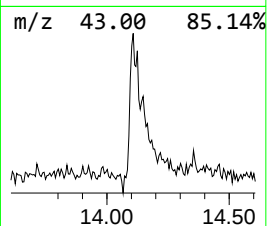
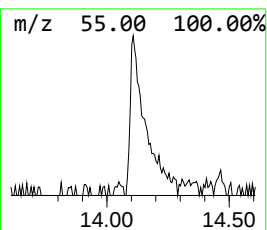
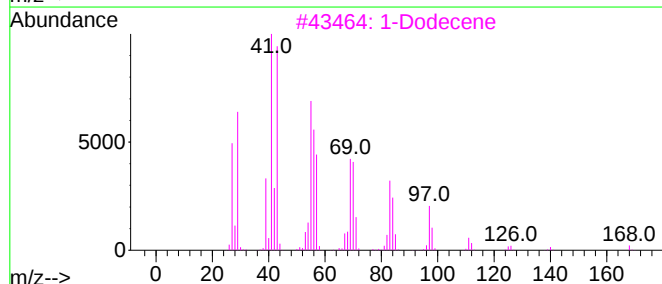
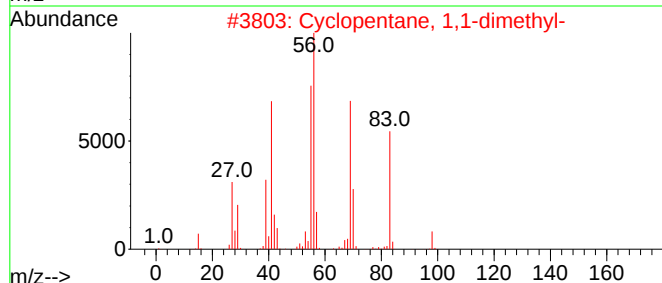
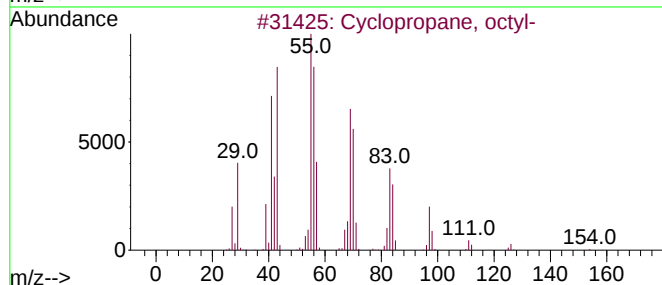
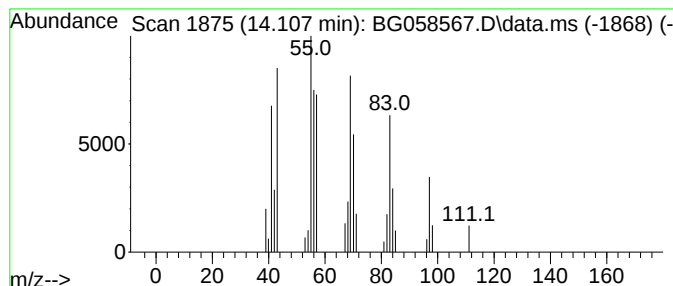
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclopropane, octyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.107	2.91 ng	103310	Acenaphthene-d10	14.460

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, octyl-	154	C11H22	001472-09-9	64
2			Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	58
3			1-Dodecene	168	C12H24	000112-41-4	53
4			1-Hexene, 3-methyl-	98	C7H14	003404-61-3	52
5			Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	50



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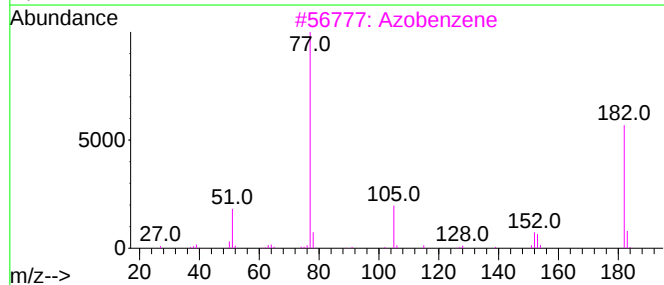
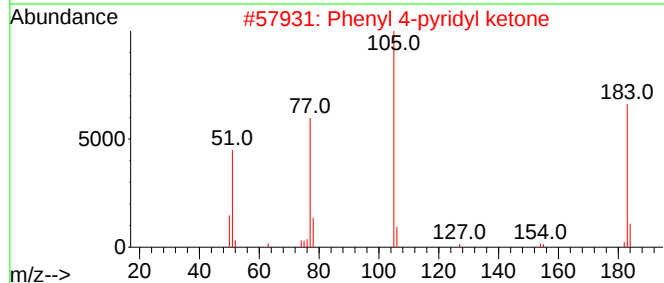
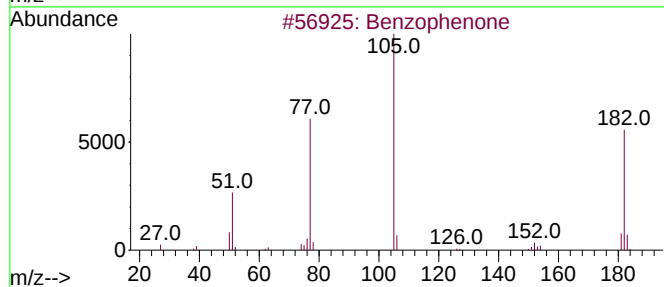
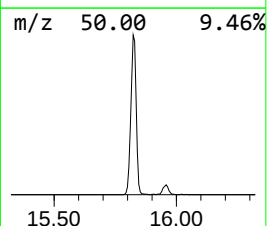
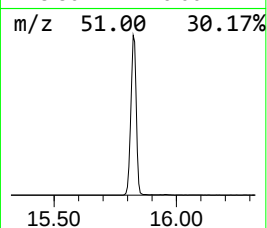
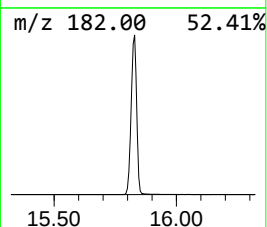
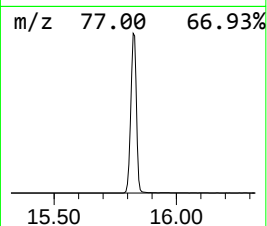
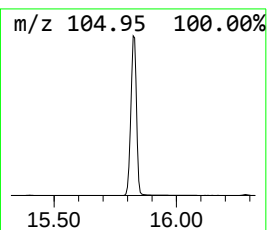
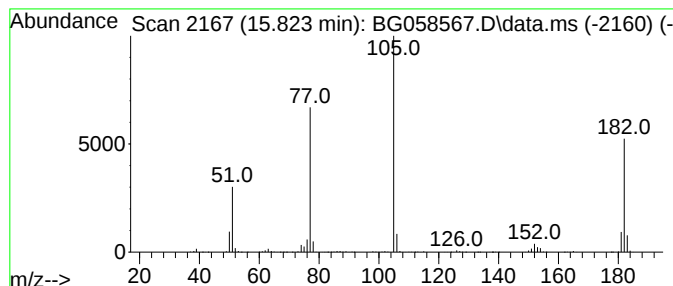
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.823	112.77 ng	4007400	Acenaphthene-d10	14.460

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3			Azobenzene	182	C12H10N2	000103-33-3	52
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47



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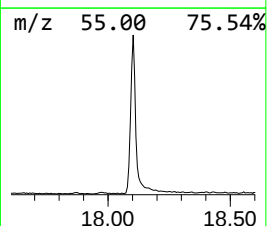
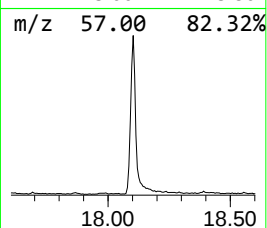
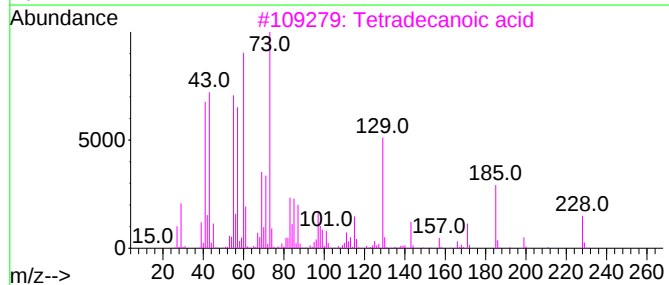
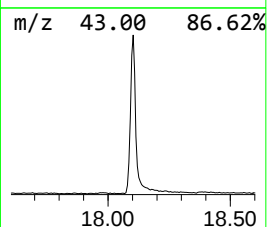
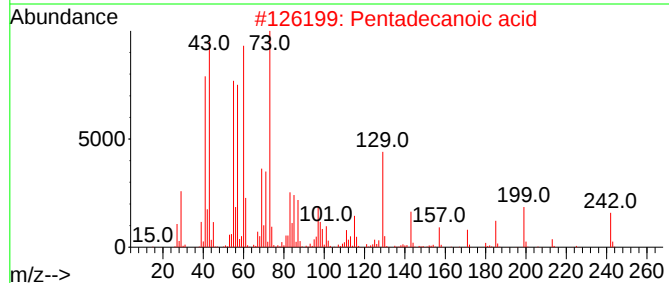
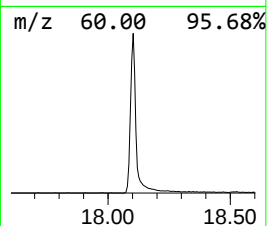
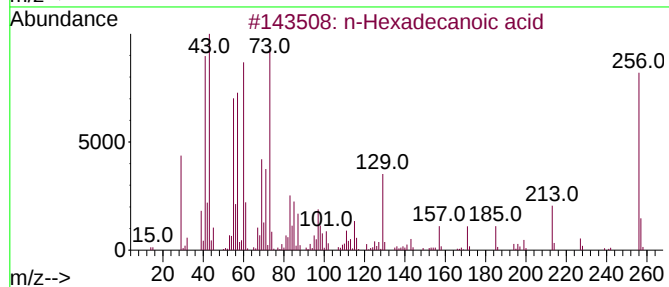
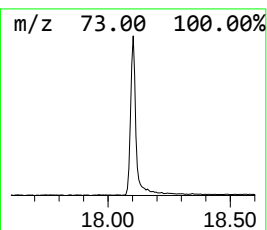
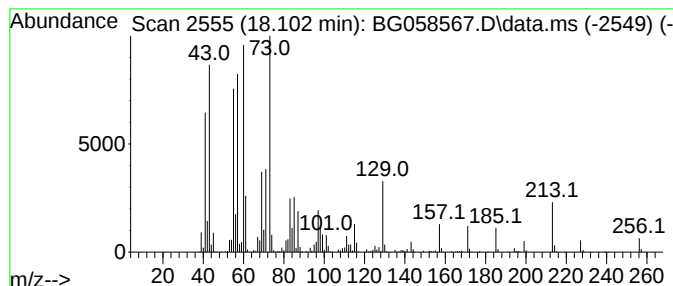
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.102	32.17 ng	1367060	Phenanthrene-d10	17.209

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Octanoic acid	144	C8H16O2	000124-07-2	43



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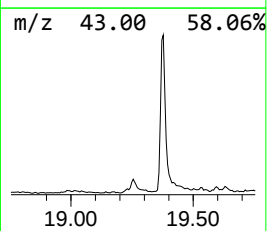
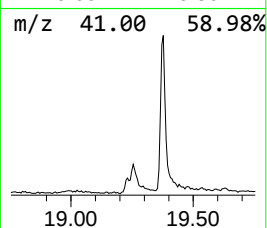
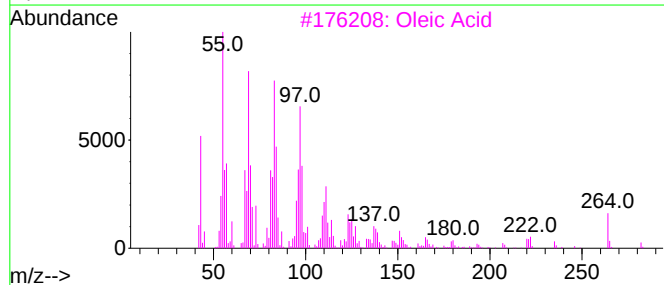
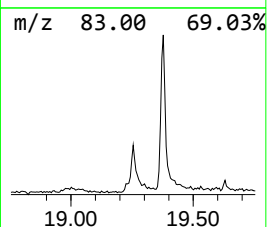
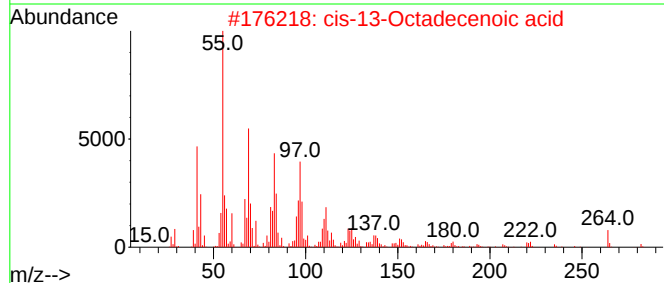
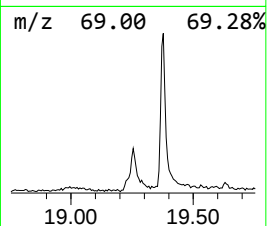
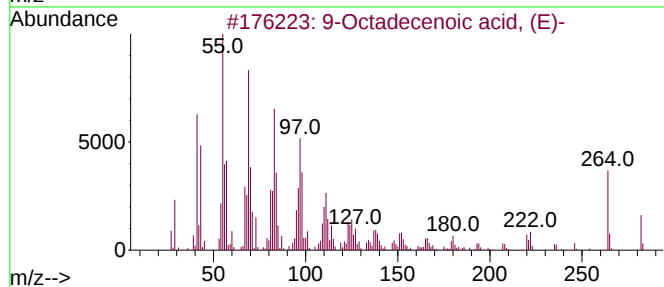
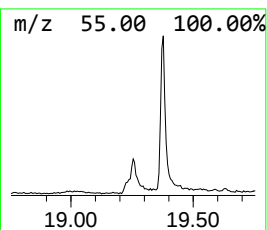
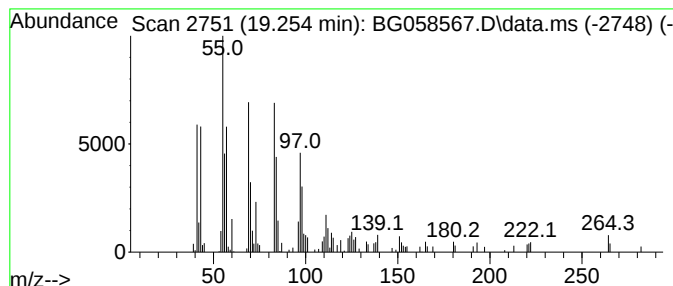
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Octadecenoic acid, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.254	4.73 ng	201129	Phenanthrene-d10	17.209

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	90
2			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	90
3			Oleic Acid	282	C18H34O2	000112-80-1	89
4			Cyclopentadecanone, 2-hydroxy-	240	C15H28O2	004727-18-8	86
5			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	83



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Data File : BG058567.D
Acq On : 1 Aug 2023 18:03
Operator : MA/JU
Sample : 03715-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

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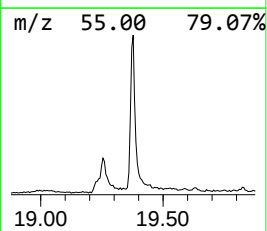
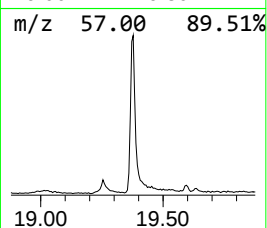
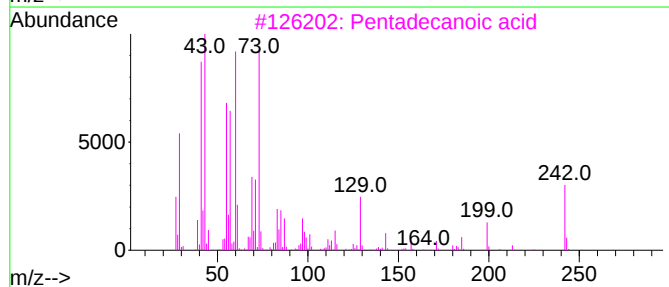
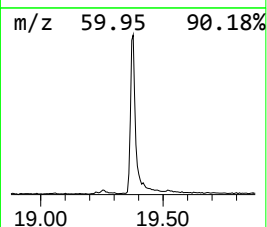
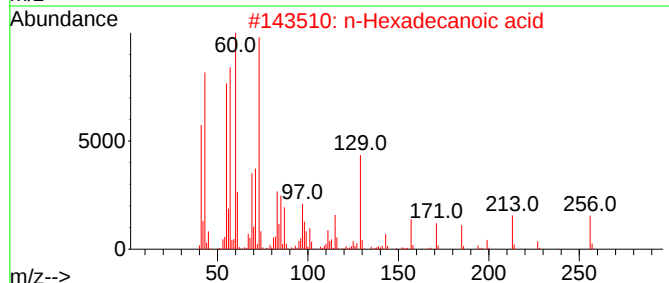
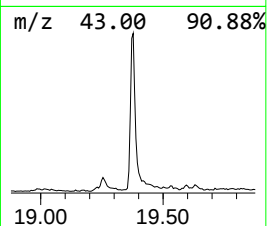
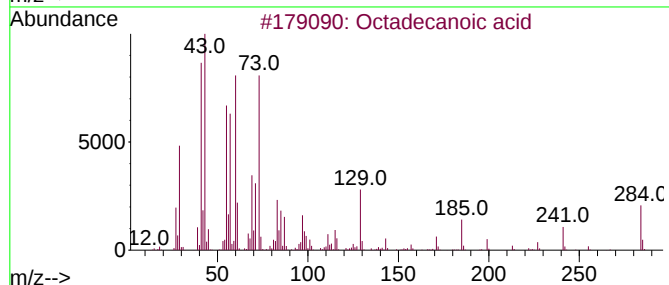
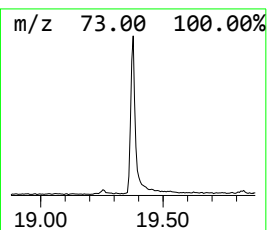
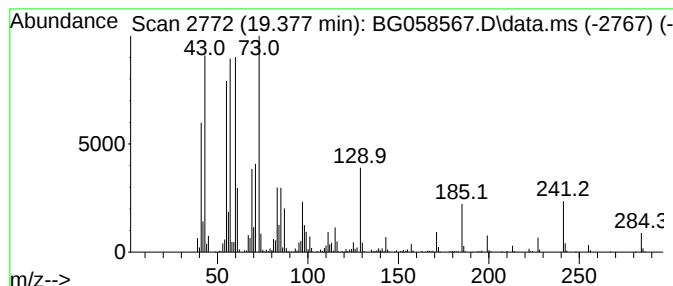
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.378	23.70 ng	1017420	Chrysene-d12	21.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058567.D
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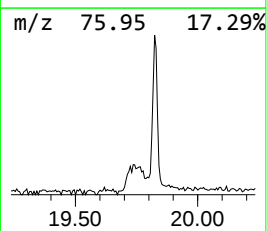
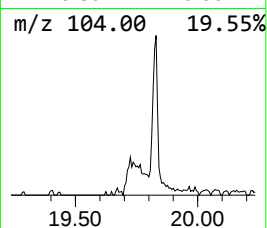
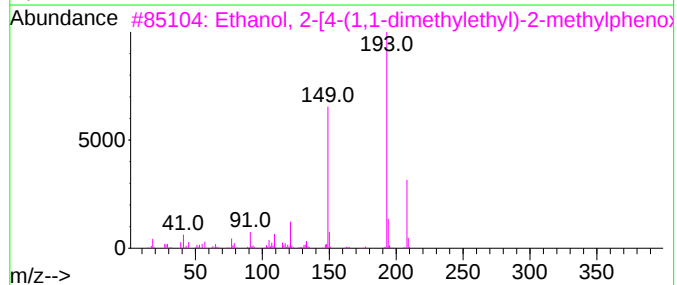
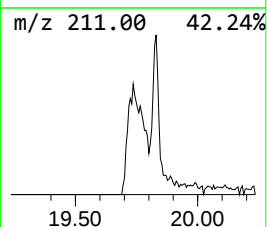
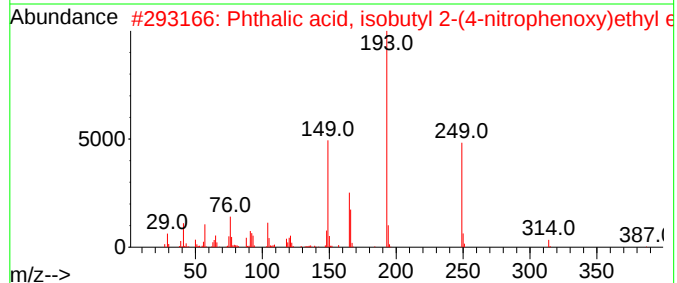
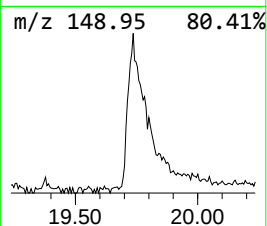
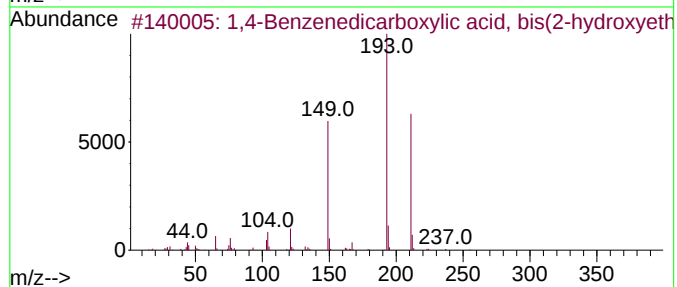
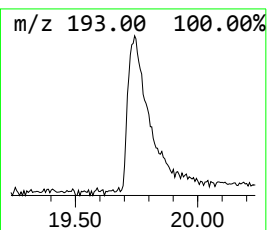
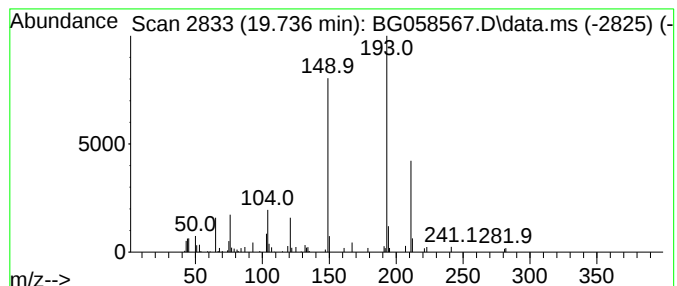
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1,4-Benzenedicarboxylic aci... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.736	3.33 ng	142958	Chrysene-d12	21.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	254	C12H14O6	000959-26-2	91
2			Phthalic acid, isobutyl 2-(4-nit...	387	C20H21NO7	1000382-57-3	59
3			Ethanol, 2-[4-(1,1-dimethylethyl...	208	C13H20O2	054934-87-1	40
4			2,4,6-Trimethoxybenzonitrile	193	C10H11NO3	002571-54-2	38
5			Phthalic acid, isobutyl 2-phenox...	342	C20H22O5	1000382-47-9	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058567.D
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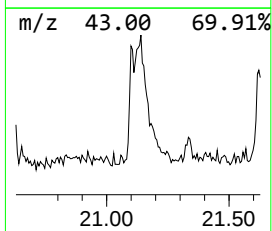
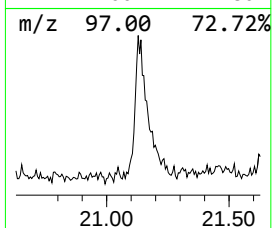
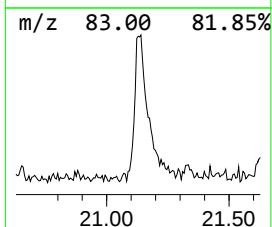
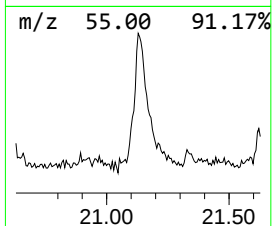
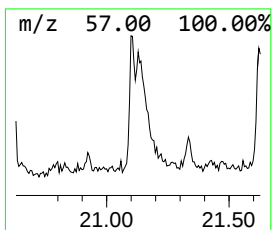
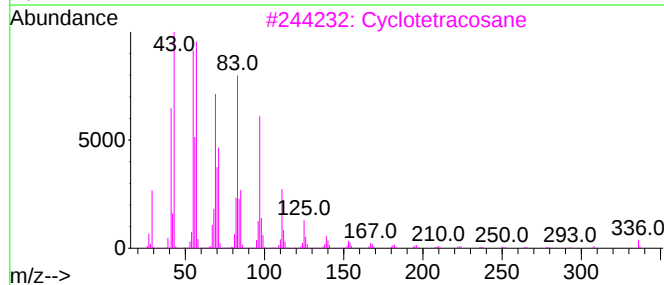
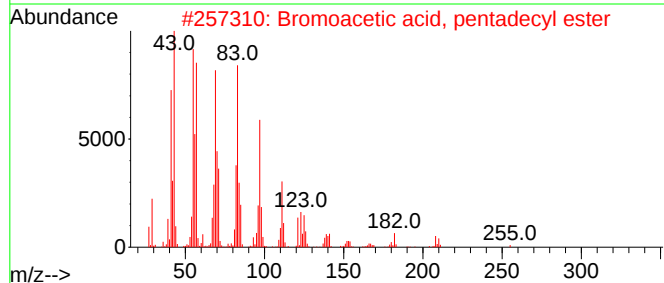
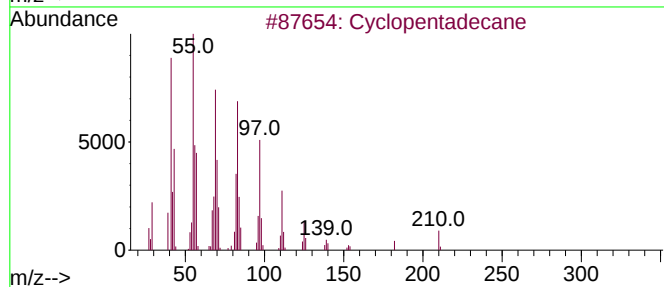
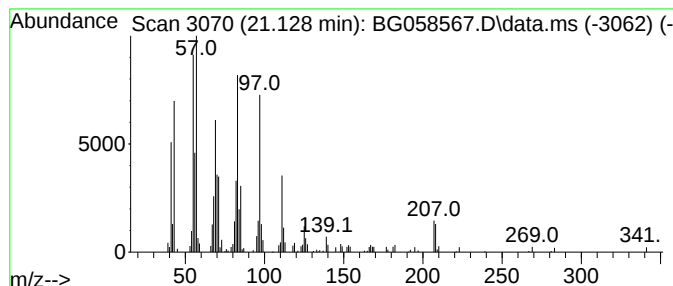
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclopentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.128	7.32 ng	314343	Chrysene-d12	21.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	95
2			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	90
3			Cyclotetracosane	336	C24H48	000297-03-0	90
4			Cyclododecane	168	C12H24	000294-62-2	89
5			1-Heptacosanol	396	C27H56O	002004-39-9	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058567.D
Acq On : 1 Aug 2023 18:03
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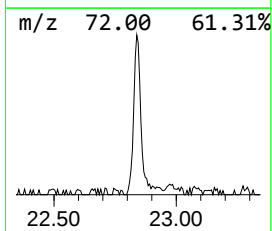
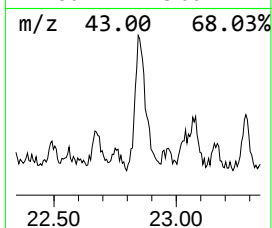
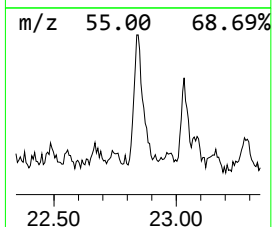
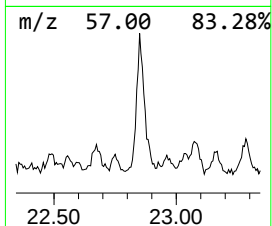
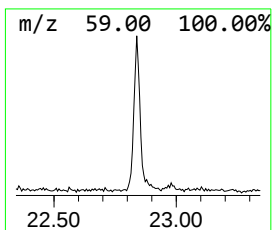
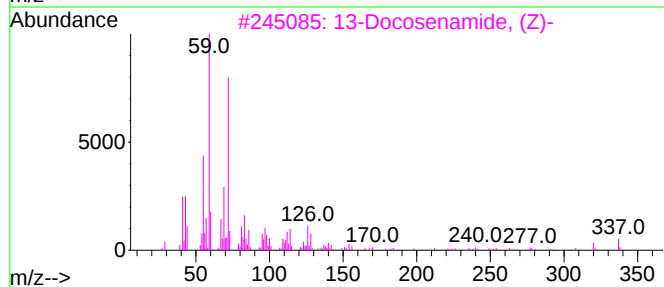
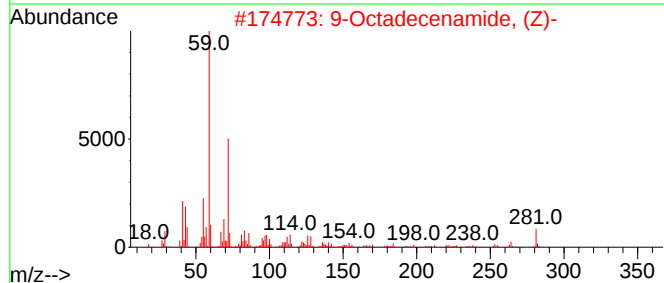
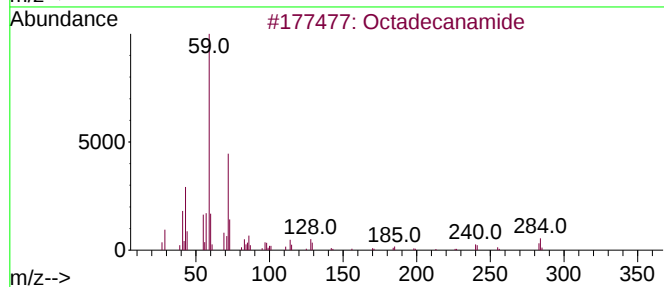
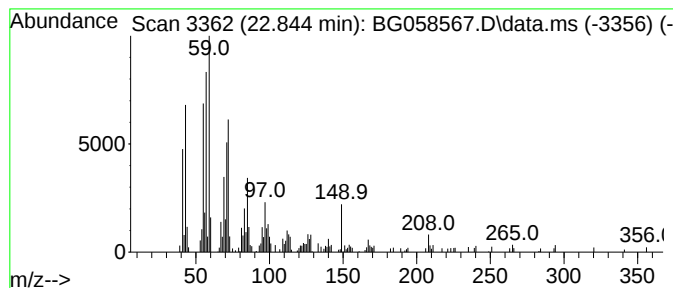
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown22.844 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.844	5.97 ng	256062	Chrysene-d12	21.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanamide	283	C18H37NO	000124-26-5	49
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	46
3			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	30
4			Heptadecane	240	C17H36	000629-78-7	25
5			Hexadecane	226	C16H34	000544-76-3	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058567.D
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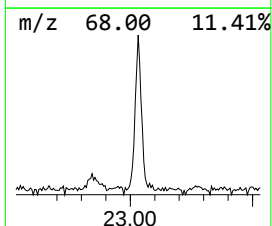
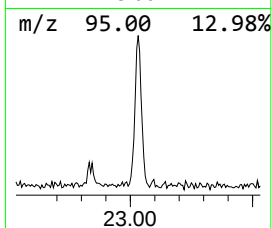
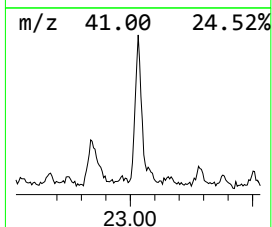
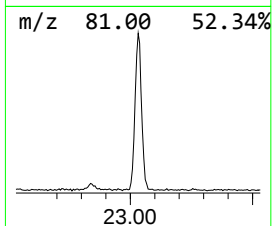
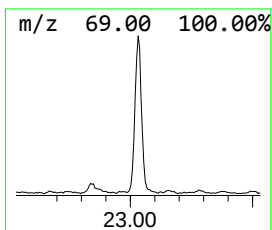
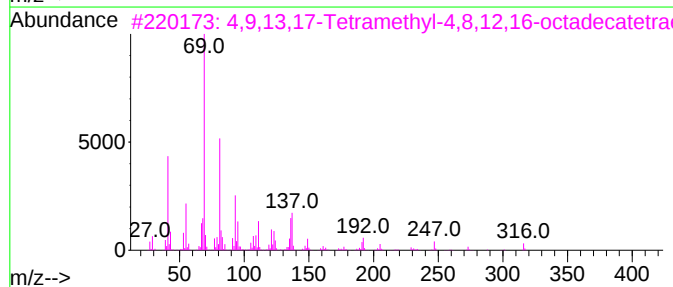
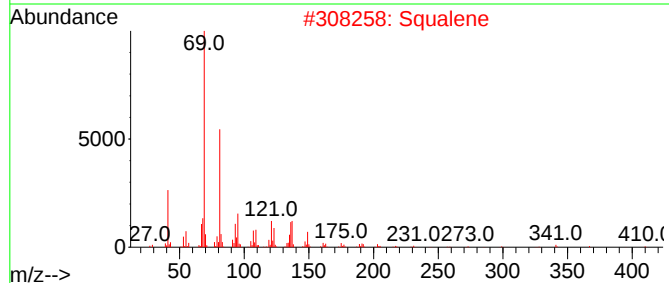
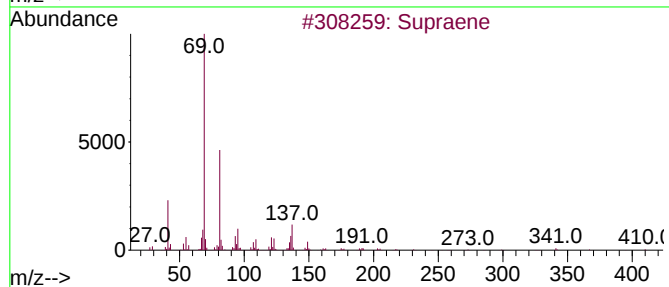
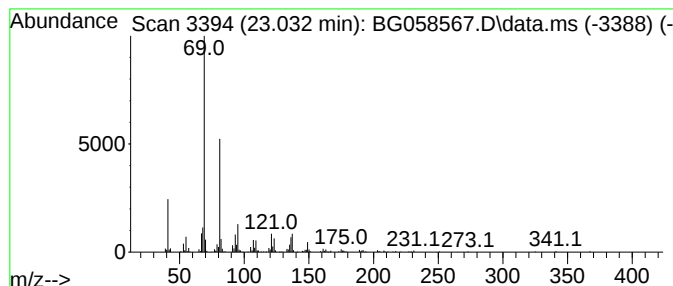
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.032	7.97 ng	410031	Perylene-d12	24.524

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	90
3			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80
5			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
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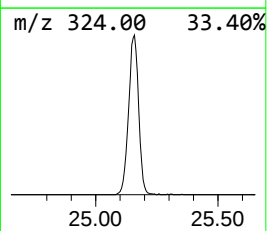
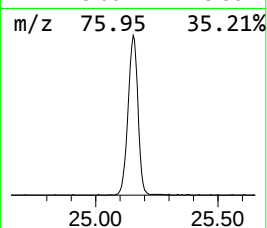
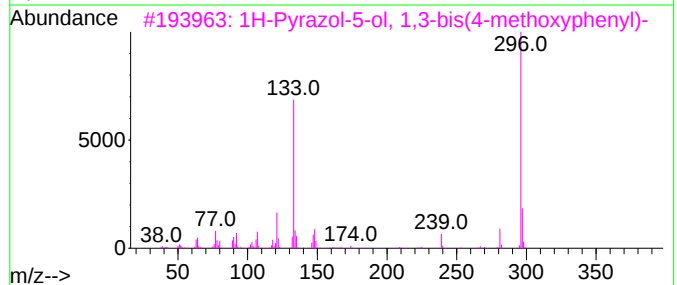
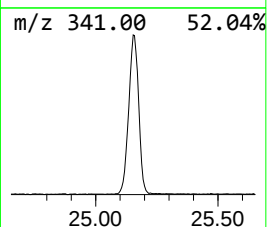
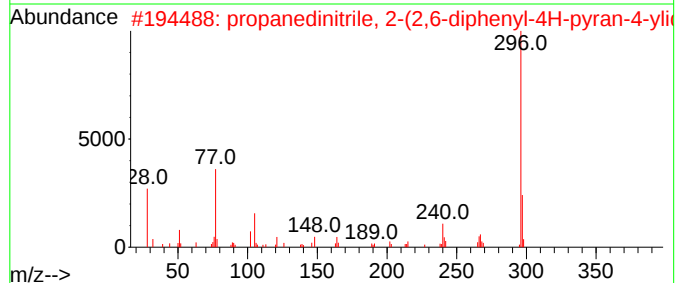
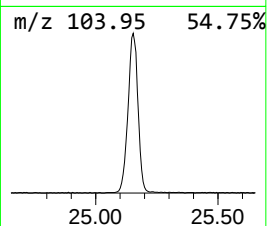
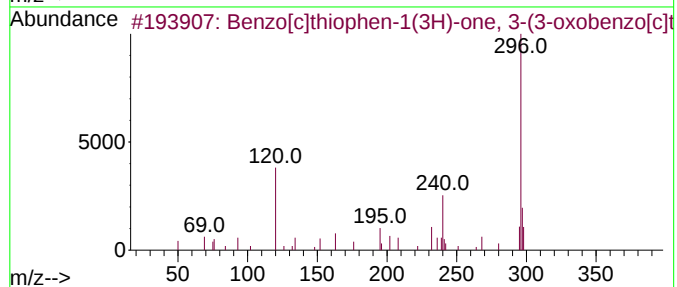
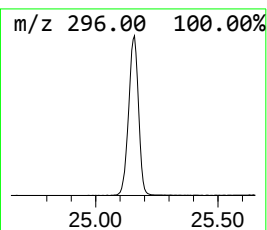
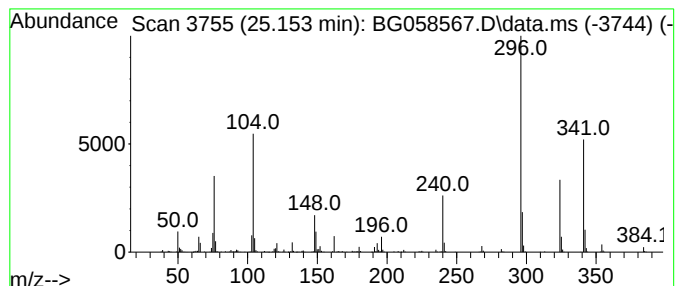
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown25.153 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.153	39.35 ng	2023640	Perylene-d12	24.524

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]thiophen-1(3H)-one, 3-(3...	296	C16H8O2S2	023667-32-5	27
2			propanedinitrile, 2-(2,6-dipheny...	296	C20H12N2O	1000402-09-2	27
3			1H-Pyrazol-5-ol, 1,3-bis(4-metho...	296	C17H16N2O3	1000337-80-1	25
4			(2S,7R,Z)-2-Ethyl-1-methyl-3-pen...	325	C20H27N3O	1000482-33-2	25
5			2-(2-Quinolyl)(1,2,4)triazolo(1...	296	C19H12N4	1000241-15-8	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058567.D
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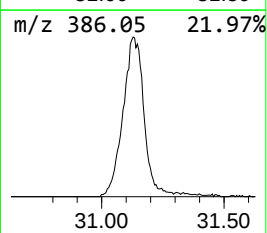
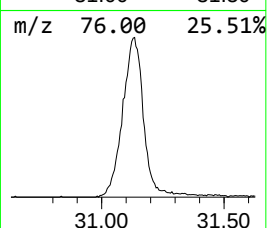
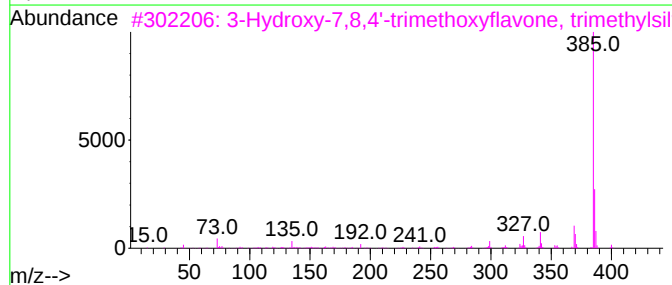
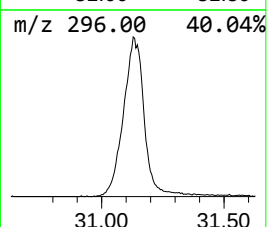
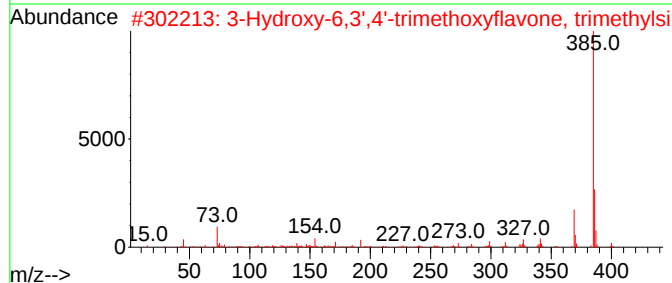
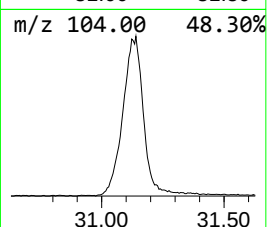
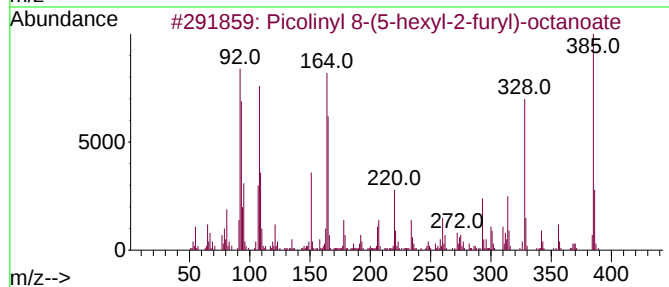
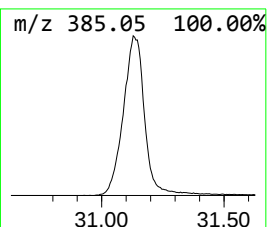
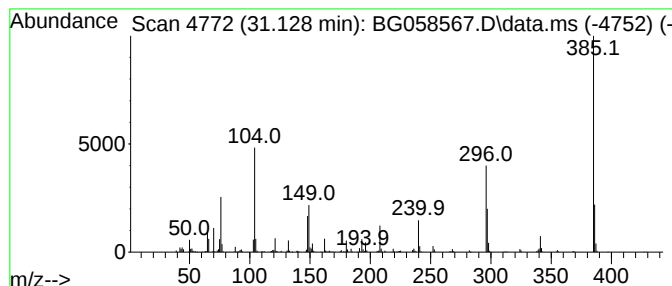
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown31.128 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.128	56.27 ng	2894200	Perylene-d12	24.524

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Picolinyl 8-(5-hexyl-2-furyl)-oc...	385	C24H35NO3	1000335-93-0	25
2			3-Hydroxy-6,3',4'-trimethoxyflav...	400	C21H24O6Si	1000448-94-7	22
3			3-Hydroxy-7,8,4'-trimethoxyflavo...	400	C21H24O6Si	1000454-18-7	22
4			2,3-Dibenzyl-5,8-dimethoxy-6-ami...	385	C24H23N3O2	056393-28-3	12
5			Silane, diethylhexyloxypentadecy...	414	C25H54O2Si	1000363-74-3	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058567.D
Acq On : 1 Aug 2023 18:03
Operator : MA/JU
Sample : 03715-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

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

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
2-Pentanone, 4-...	4.912	3.8	ng	62669	1	7.815	331014	20.0
Cyclopropane, o...	14.107	2.9	ng	103310	3	14.460	710712	20.0
Benzophenone	15.823	112.8	ng	4007400	3	14.460	710712	20.0
n-Hexadecanoic ...	18.102	32.2	ng	1367060	4	17.209	849806	20.0
9-Octadecenoic ...	19.254	4.7	ng	201129	4	17.209	849806	20.0
Octadecanoic acid	19.378	23.7	ng	1017420	5	21.451	858432	20.0
1,4-Benzenedica...	19.736	3.3	ng	142958	5	21.451	858432	20.0
Cyclopentadecane	21.128	7.3	ng	314343	5	21.451	858432	20.0
unknown22.844	22.844	6.0	ng	256062	5	21.451	858432	20.0
Supraene	23.032	8.0	ng	410031	6	24.524	1028650	20.0
unknown25.153	25.153	39.4	ng	2023640	6	24.524	1028650	20.0
unknown31.128	31.128	56.3	ng	2894200	6	24.524	1028650	20.0