

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031125\
 Data File : BG064096.D
 Acq On : 11 Mar 2025 15:16
 Operator : RC/JU
 Sample : Q1534-19
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 OR-363-COMP-19

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-BG030525.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG064096.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.456	396	403	411	rBV	541561	869218	48.40%	7.759%
2	7.030	663	671	679	rBV	586221	985933	54.89%	8.801%
3	7.864	806	813	820	rBV	154323	252166	14.04%	2.251%
4	9.016	1000	1009	1020	rBV	341604	596176	33.19%	5.322%
5	9.574	1098	1104	1113	rVB3	17515	30512	1.70%	0.272%
6	10.649	1279	1287	1295	rBV	196933	349834	19.48%	3.123%
7	13.111	1699	1706	1715	rBB	822915	1224764	68.19%	10.933%
8	14.486	1933	1940	1947	rVB	314058	475402	26.47%	4.244%
9	15.843	2165	2171	2178	rBV	159378	220023	12.25%	1.964%
10	15.967	2184	2192	2204	rBV	664872	1020893	56.84%	9.113%
11	17.224	2400	2406	2411	rBV2	375901	575791	32.06%	5.140%
12	17.265	2411	2413	2418	rVB	24801	29027	1.62%	0.259%
13	18.129	2552	2560	2570	rBV	187687	308592	17.18%	2.755%
14	19.275	2750	2755	2761	rBV	65026	94187	5.24%	0.841%
15	19.404	2772	2777	2779	rBV	52840	68182	3.80%	0.609%
16	19.427	2779	2781	2787	rVB4	51041	54816	3.05%	0.489%
17	19.592	2804	2809	2812	rBV5	44385	69458	3.87%	0.620%
18	19.633	2812	2816	2821	rVB	51055	91469	5.09%	0.817%
19	19.756	2834	2837	2844	rVB9	12080	18881	1.05%	0.169%
20	19.845	2844	2852	2863	rBV	1358021	1796084	100.00%	16.033%
21	20.620	2978	2984	2986	rBV4	14677	18764	1.04%	0.167%
22	21.137	3068	3072	3079	rBV4	119215	179341	9.99%	1.601%
23	21.454	3119	3126	3131	rBV	416119	687099	38.26%	6.133%
24	21.496	3131	3133	3139	rVB2	34459	49400	2.75%	0.441%
25	22.259	3259	3263	3267	rVB6	12686	20272	1.13%	0.181%
26	22.865	3362	3366	3377	rBV4	51539	99689	5.55%	0.890%
27	23.076	3396	3402	3408	rBV2	48281	91573	5.10%	0.817%
28	23.528	3468	3479	3484	rBV4	26234	88373	4.92%	0.789%
29	23.658	3495	3501	3505	rBV9	17405	36368	2.02%	0.325%
30	23.705	3505	3509	3514	rVB6	15983	34299	1.91%	0.306%
31	24.181	3585	3590	3592	rBV2	15593	24796	1.38%	0.221%
32	24.328	3609	3615	3622	rVB4	15322	35255	1.96%	0.315%
33	24.469	3630	3639	3648	rBV2	243527	637394	35.49%	5.690%
34	25.591	3824	3830	3837	rBV6	13128	37806	2.10%	0.337%
35	25.697	3841	3848	3849	rBV6	18886	30692	1.71%	0.274%

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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-BG030525.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

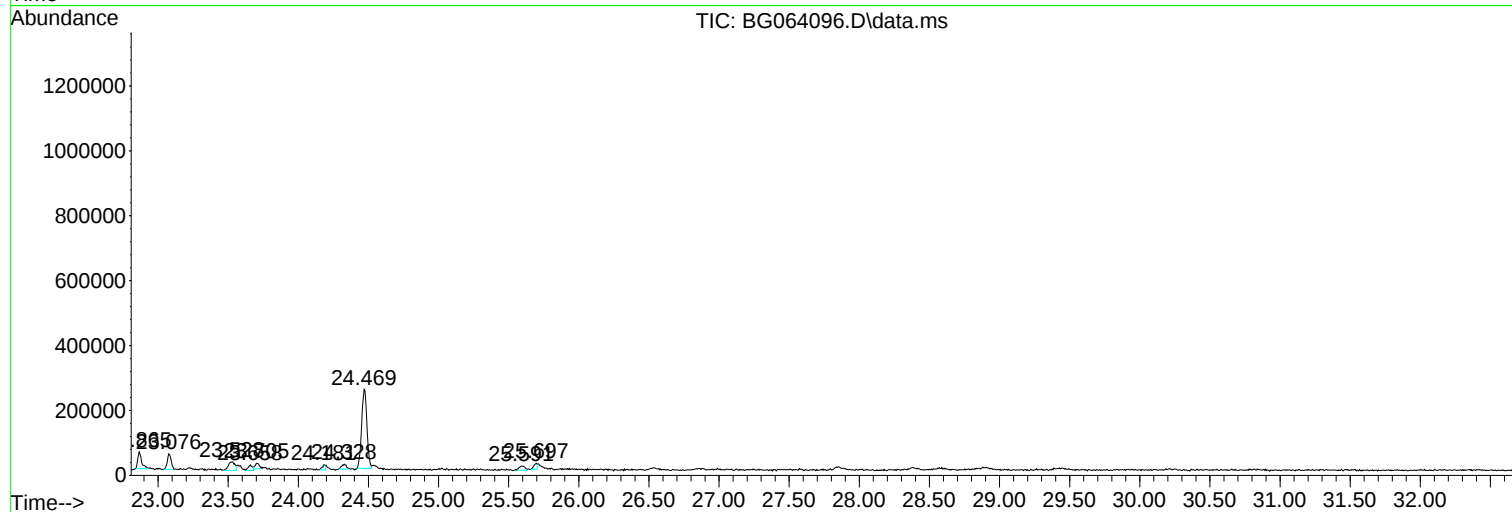
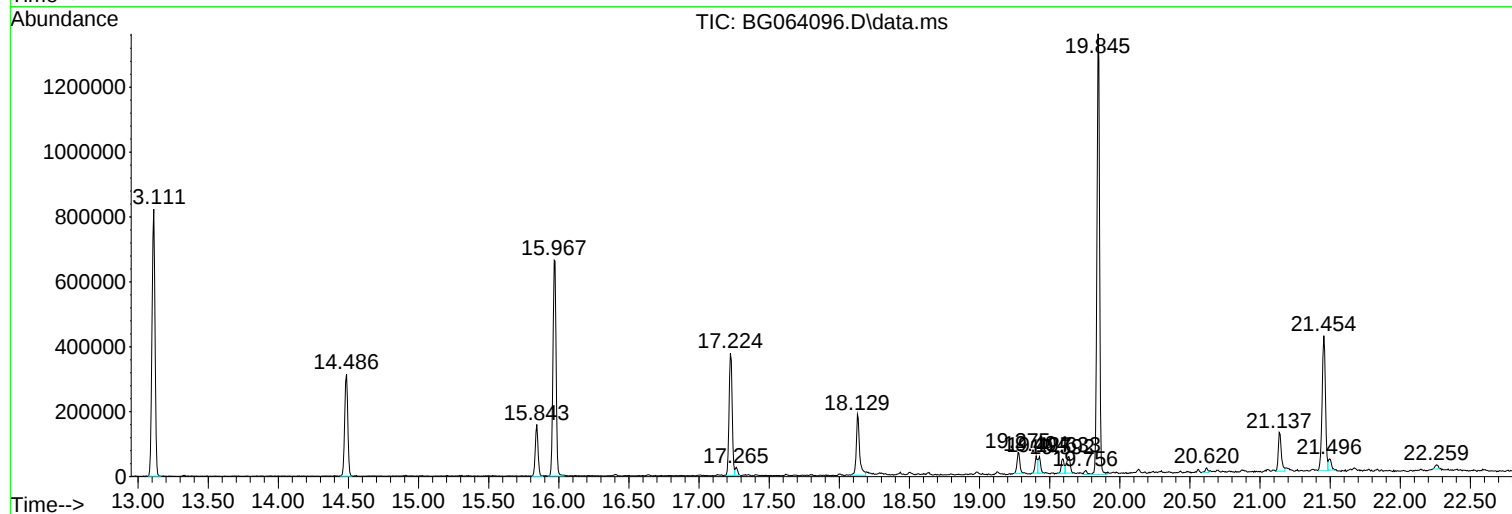
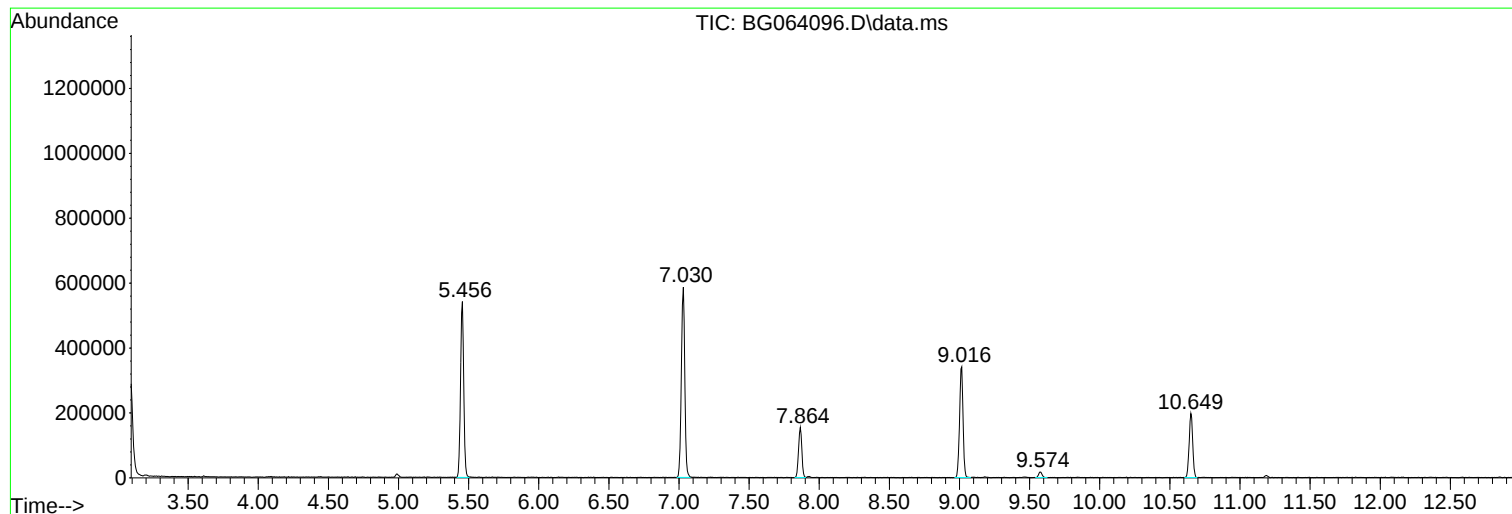
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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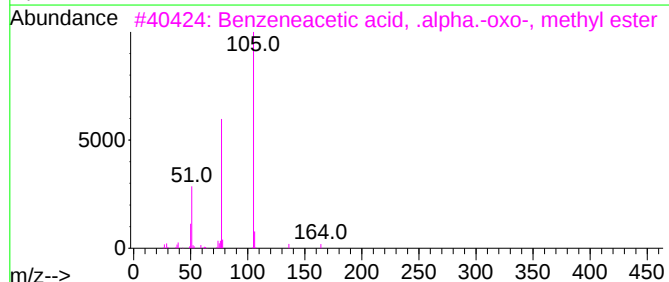
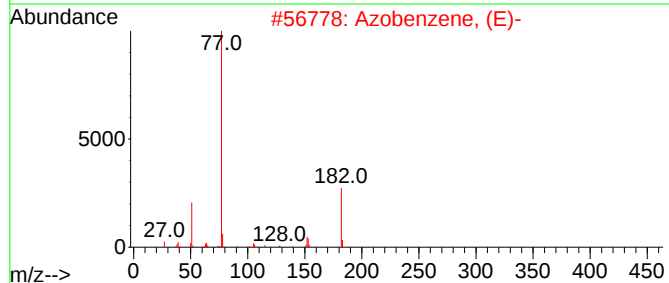
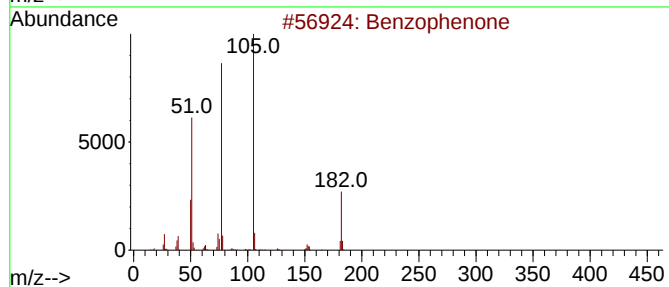
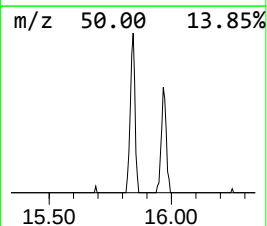
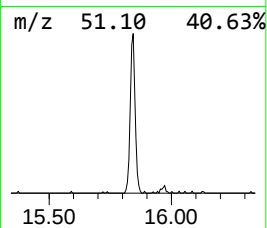
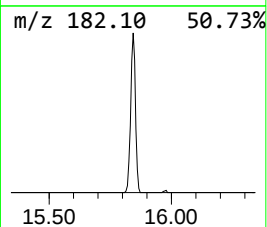
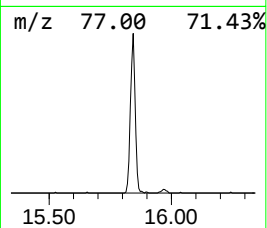
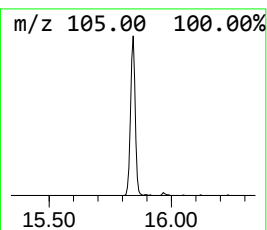
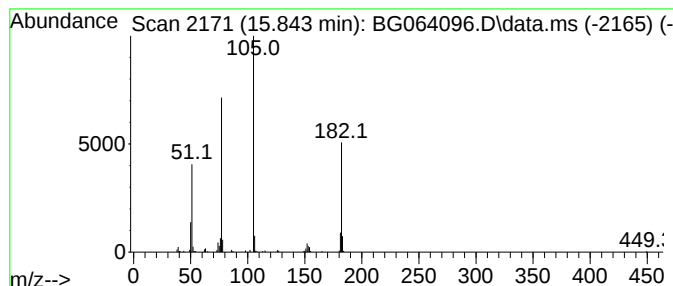
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.843	9.26 ng	220023	Acenaphthene-d10	14.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Azobenzene, (E)-	182	C12H10N2	017082-12-1	59
3			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	52
4			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	50
5			2-Pyrazoline-3-carbonitrile, 1-b...	199	C11H9N3O	067872-68-8	50



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Sample : Q1534-19
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-363-COMP-19

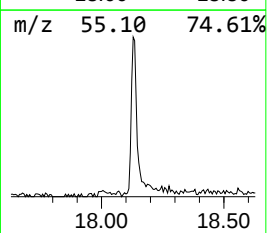
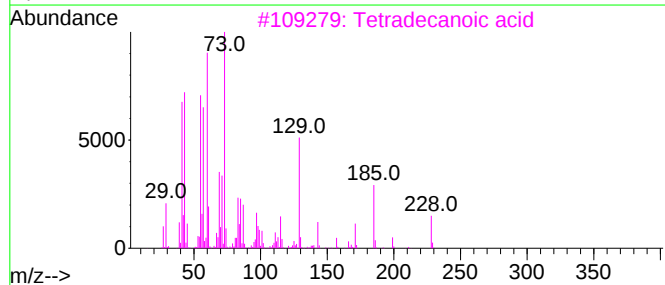
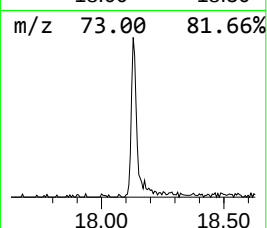
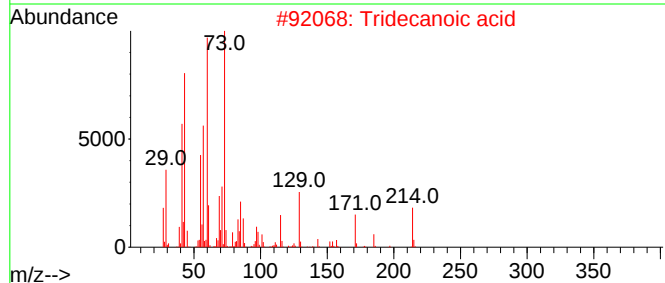
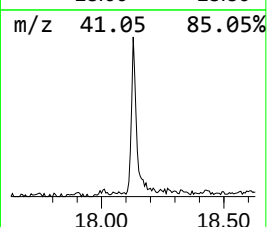
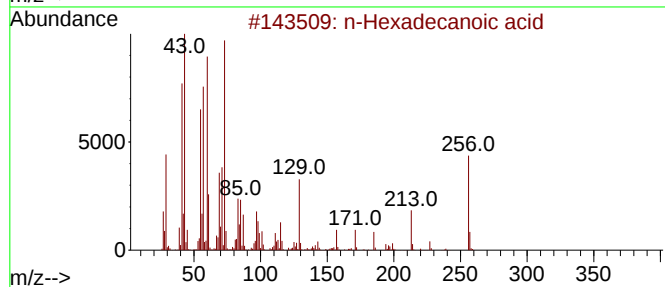
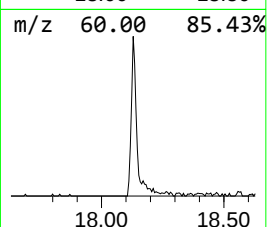
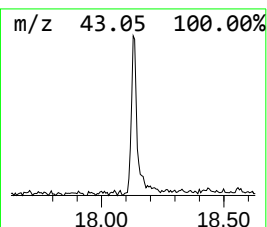
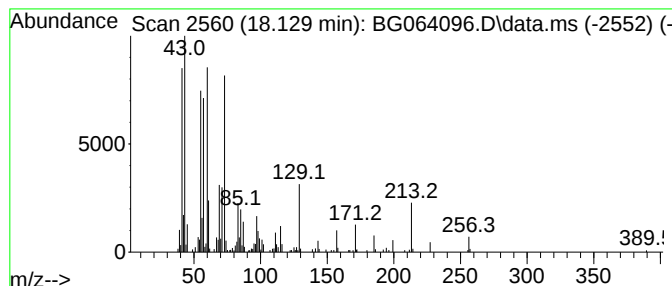
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.129	10.72 ng	308592	Phenanthrene-d10	17.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2			Tridecanoic acid	214	C13H26O2	000638-53-9	68
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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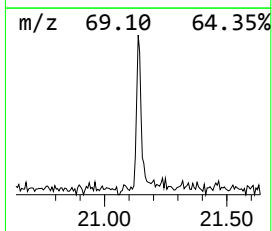
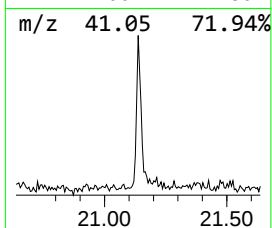
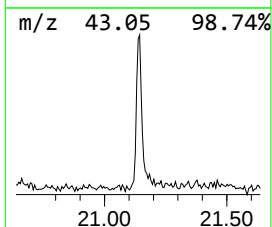
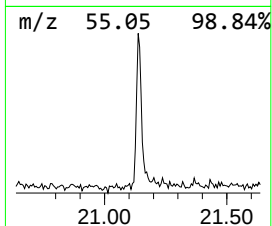
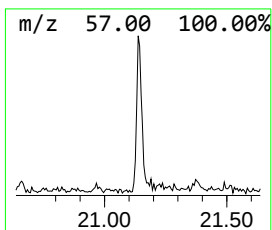
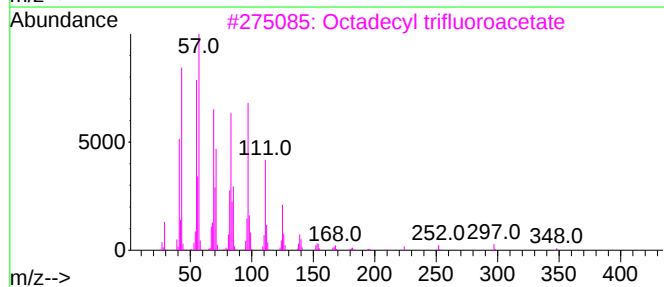
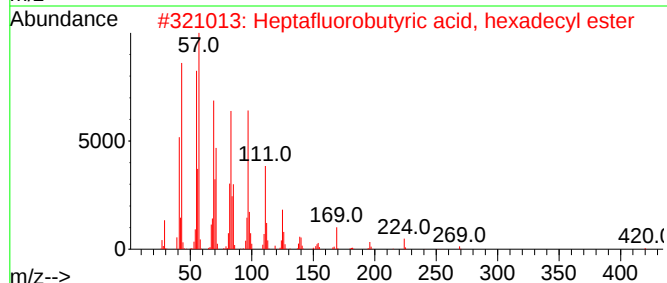
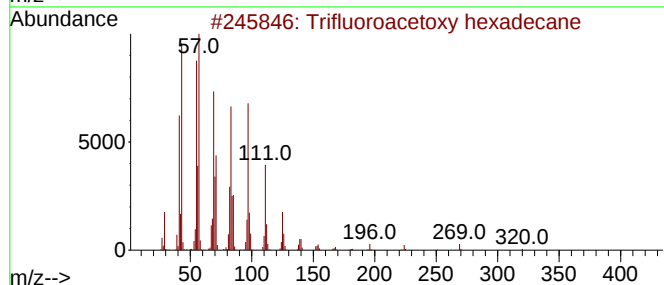
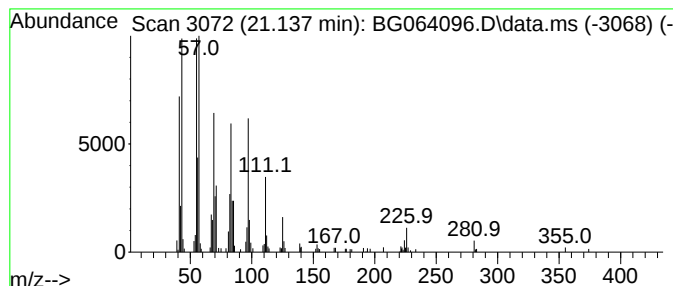
Instrument :
BNA_G
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.137	5.22 ng	179341	Chrysene-d12	21.454	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	87
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	87
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	87
5	3-Hexadecene, (Z)-	224	C16H32	034303-81-6	86



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Misc :
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Instrument :
BNA_G
ClientSampleId :
OR-363-COMP-19

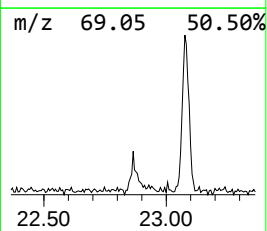
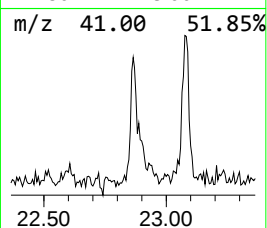
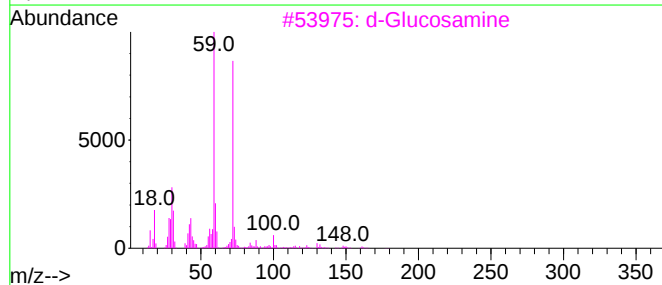
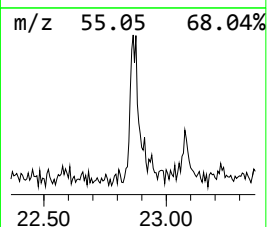
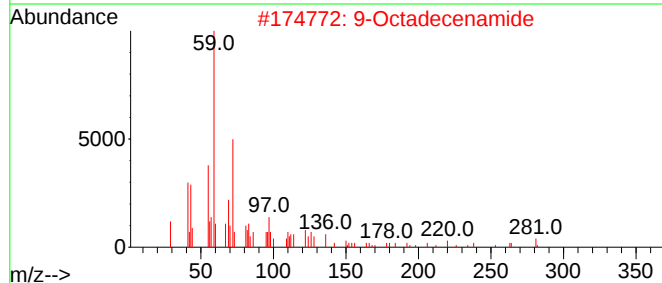
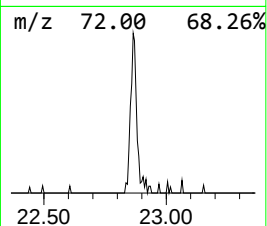
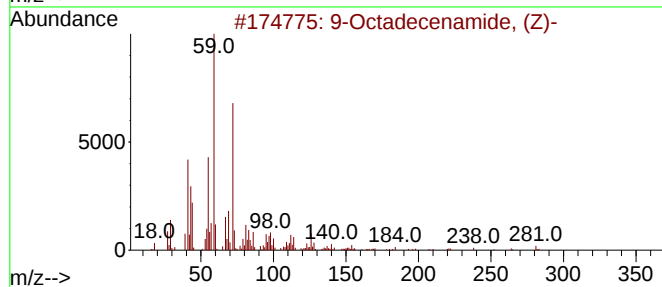
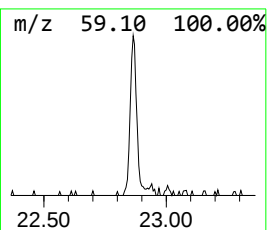
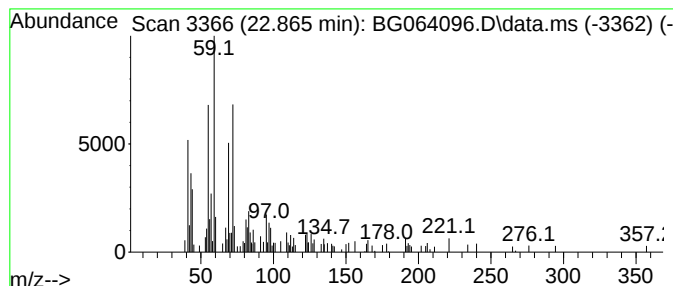
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.865	2.90 ng	99689	Chrysene-d12	21.454

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	74
2			9-Octadecenamide	281	C18H35NO	003322-62-1	59
3			d-Glucosamine	179	C6H13NO5	000090-77-7	50
4			Tetradecanamide	227	C14H29NO	000638-58-4	47
5			Palmitoleamide	253	C16H31NO	106010-22-4	43



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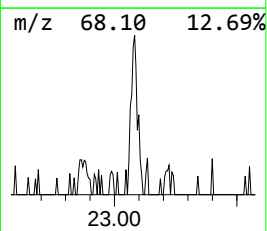
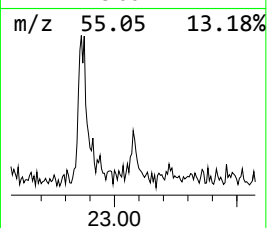
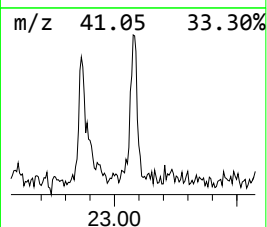
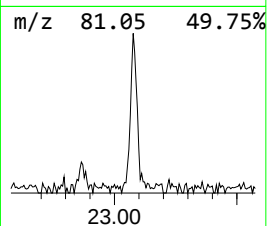
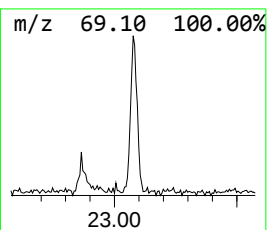
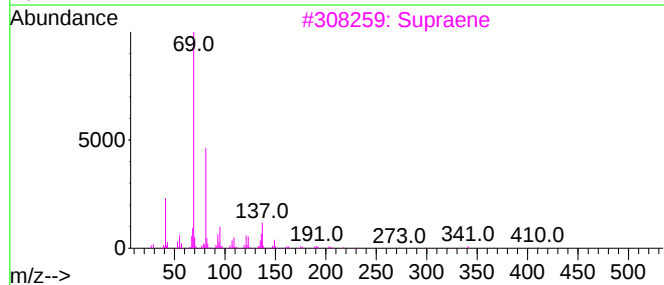
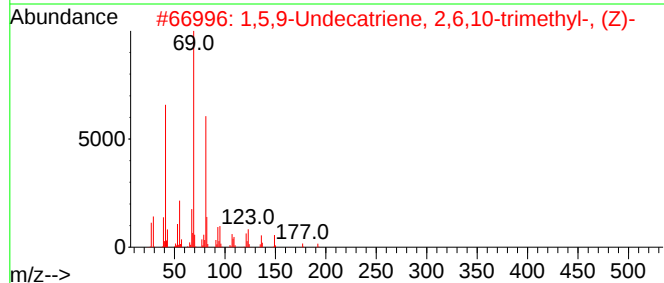
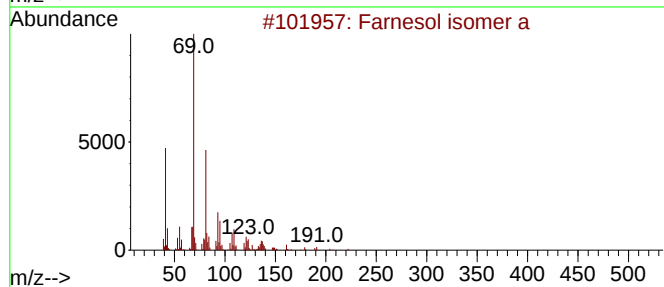
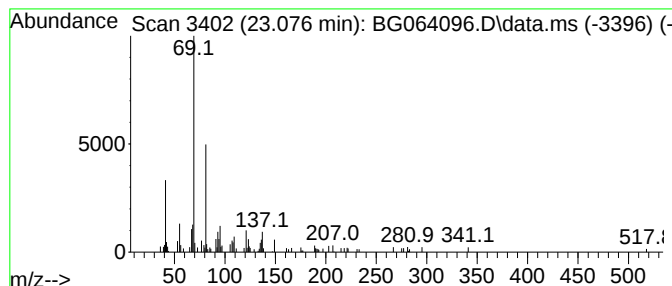
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Farnesol isomer a Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.076	2.87 ng	91573	Perylene-d12	24.469

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Farnesol isomer a	222	C15H26O	1000108-92-4	83
2		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	76
3		Supraene	410	C30H50	007683-64-9	74
4		trans-Farnesol	222	C15H26O	000106-28-5	70
5		(2E,6E,10E)-3,7,11,15-Tetramethy...	318	C21H34O2	125456-63-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031125\
Data File : BG064096.D
Acq On : 11 Mar 2025 15:16
Operator : RC/JU
Sample : Q1534-19
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-363-COMP-19

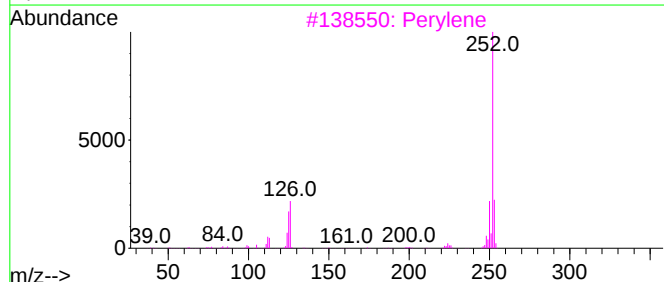
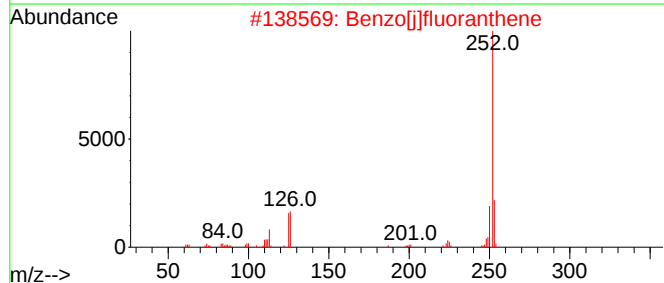
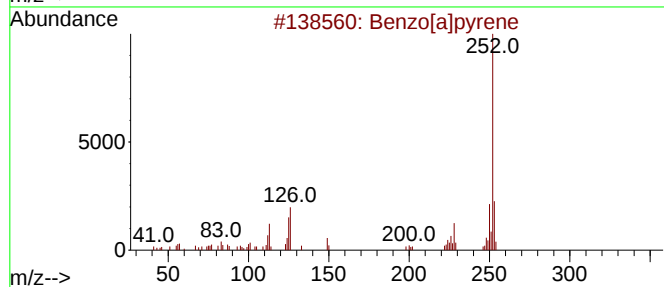
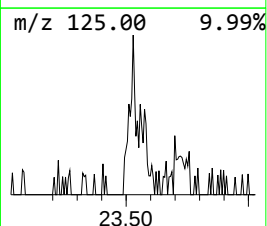
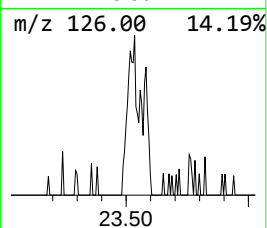
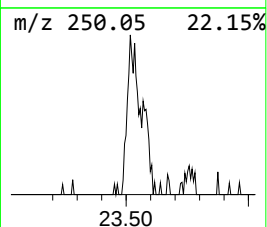
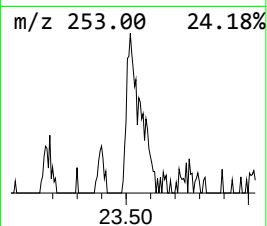
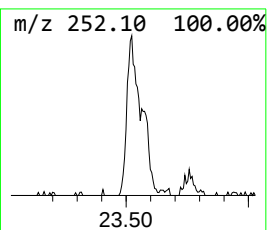
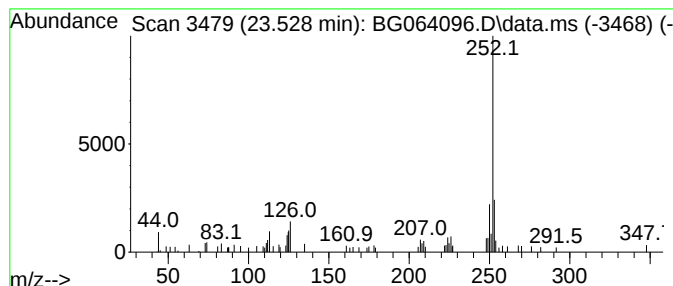
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[j]fluoranthene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.529	2.77 ng	88373	Perylene-d12	24.469

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene	252	C20H12	000050-32-8	95
2			Benzo[j]fluoranthene	252	C20H12	000205-82-3	90
3			Perylene	252	C20H12	000198-55-0	81
4			Benzo[e]pyrene	252	C20H12	000192-97-2	81
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031125\
Data File : BG064096.D
Acq On : 11 Mar 2025 15:16
Operator : RC/JU
Sample : Q1534-19
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-363-COMP-19

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.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	15.843	9.3	ng	220023	3	14.486	475402	20.0
n-Hexadecanoic ...	18.129	10.7	ng	308592	4	17.224	575791	20.0
Trifluoroacetox...	21.137	5.2	ng	179341	5	21.454	687099	20.0
9-Octadecenamid...	22.865	2.9	ng	99689	5	21.454	687099	20.0
Farnesol isomer a	23.076	2.9	ng	91573	6	24.469	637394	20.0
Benzo[j]fluoran...	23.529	2.8	ng	88373	6	24.469	637394	20.0