

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM050125\
 Data File : BM050071.D
 Acq On : 01 May 2025 19:20
 Operator : RC/JU
 Sample : Q1914-03
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SS-2

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-BM042825.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM050071.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.869	314	320	330	rBV	248866	369121	4.01%	0.623%
2	5.340	393	400	420	rBV	2435719	3699263	40.16%	6.241%
3	6.934	663	671	695	rBV	2309983	4031519	43.76%	6.802%
4	7.745	801	809	819	rBV	948482	1506429	16.35%	2.542%
5	8.904	999	1006	1015	rBV	1360156	2356913	25.59%	3.976%
6	10.539	1272	1284	1300	rBV	1096347	2101058	22.81%	3.545%
7	11.969	1519	1527	1533	rBV	116696	195715	2.12%	0.330%
8	13.010	1697	1704	1715	rBV	3982275	5840701	63.40%	9.854%
9	13.222	1735	1740	1748	rVB	158556	227147	2.47%	0.383%
10	14.122	1889	1893	1901	rBV	60814	112958	1.23%	0.191%
11	14.222	1907	1910	1917	rVB2	69993	113080	1.23%	0.191%
12	14.298	1918	1923	1927	rBV	240486	318429	3.46%	0.537%
13	14.392	1930	1939	1947	rVV	1899419	2861401	31.06%	4.828%
14	14.916	2025	2028	2036	rVB5	56127	95739	1.04%	0.162%
15	15.251	2081	2085	2089	rVB	237056	281556	3.06%	0.475%
16	15.657	2151	2154	2158	rVB	82013	109139	1.18%	0.184%
17	15.751	2165	2170	2176	rBV	435661	638320	6.93%	1.077%
18	15.886	2187	2193	2210	rBV	3688908	5453129	59.20%	9.200%
19	16.110	2227	2231	2234	rBV	272494	367722	3.99%	0.620%
20	16.904	2362	2366	2370	rBV	218709	267188	2.90%	0.451%
21	16.957	2371	2375	2385	rVB2	109058	202932	2.20%	0.342%
22	17.139	2401	2406	2411	rBV2	2351907	3346563	36.33%	5.646%
23	17.186	2411	2414	2420	rVB	282421	389006	4.22%	0.656%
24	17.280	2426	2430	2434	rVB	107107	156490	1.70%	0.264%
25	17.557	2474	2477	2486	rVB2	57289	107057	1.16%	0.181%
26	17.639	2487	2491	2497	rVB	205801	249985	2.71%	0.422%
27	17.815	2518	2521	2527	rVB	73314	92881	1.01%	0.157%
28	18.039	2553	2559	2568	rBV2	566412	1025348	11.13%	1.730%
29	18.215	2585	2589	2593	rBV3	64686	108656	1.18%	0.183%
30	18.333	2605	2609	2614	rBV	190601	248763	2.70%	0.420%
31	18.957	2709	2715	2719	rBV3	331288	573991	6.23%	0.968%
32	18.992	2719	2721	2726	rVB5	183616	193643	2.10%	0.327%
33	19.204	2752	2757	2764	rBV	775630	1071878	11.64%	1.808%
34	19.321	2773	2777	2781	rBV4	123476	200341	2.17%	0.338%
35	19.562	2810	2818	2828	rVB	694068	1265620	13.74%	2.135%
36	19.768	2847	2853	2858	rBV	8309138	9211744	100.00%	15.542%

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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_M\Methods\8270-BM042825.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.062	2900	2903	2910	rVB2	152053	285127	3.10%	0.481%
38	21.062	3069	3073	3080	rBV5	295309	491504	5.34%	0.829%
39	21.380	3120	3127	3132	rBV2	2854260	4570509	49.62%	7.711%
40	21.427	3132	3135	3146	rVB	413924	676338	7.34%	1.141%
41	21.521	3148	3151	3155	rBV	207540	255194	2.77%	0.431%
42	24.374	3628	3636	3644	rVB	1498768	3600998	39.09%	6.075%

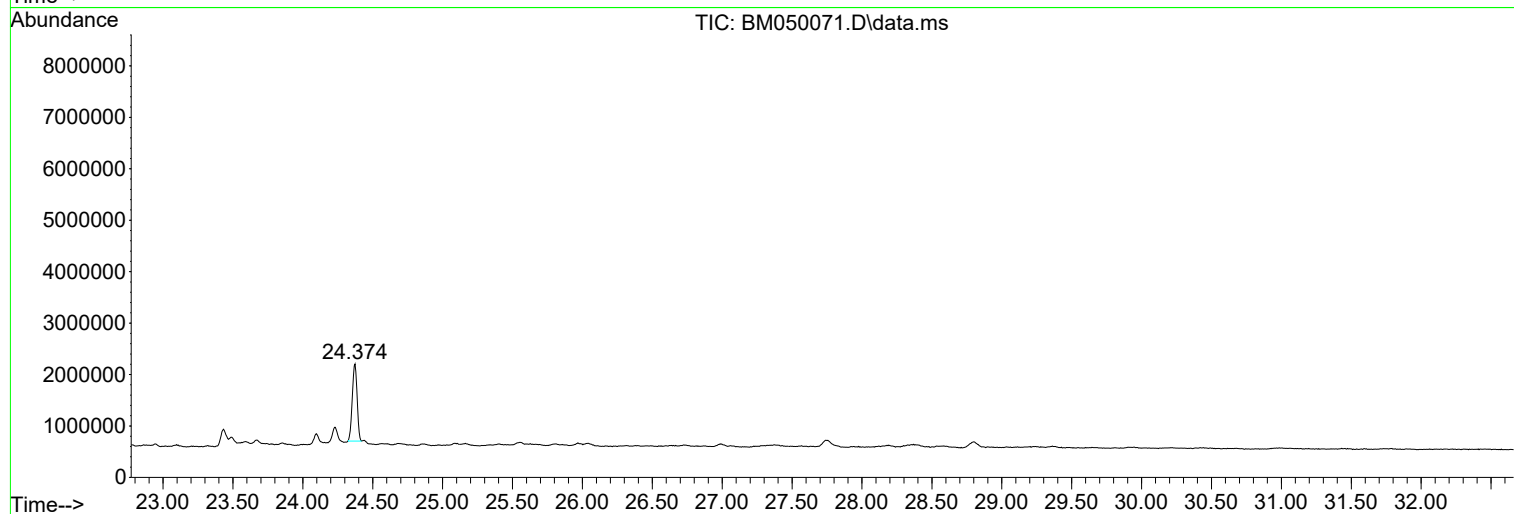
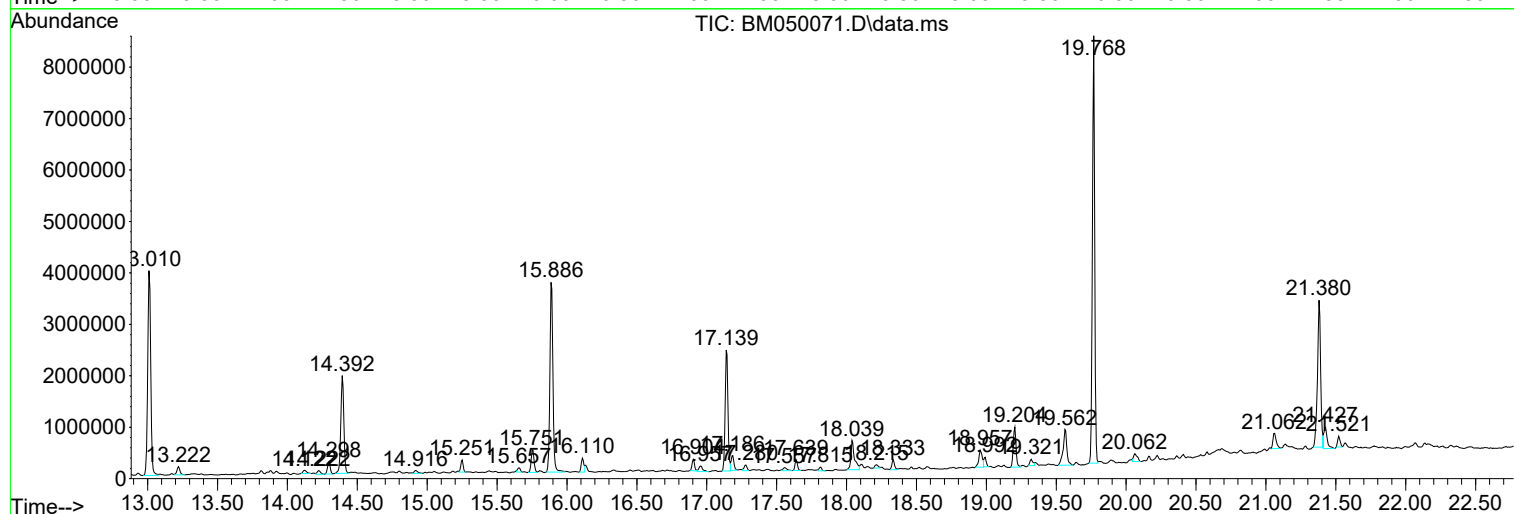
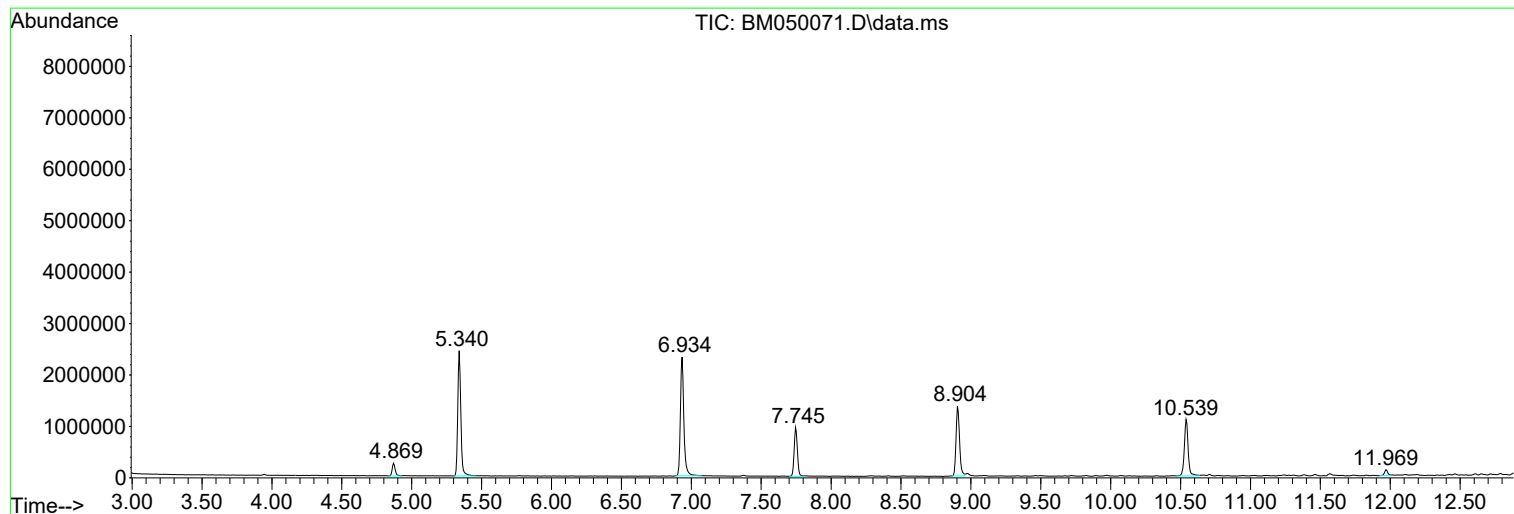
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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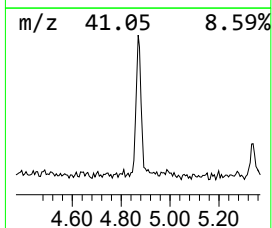
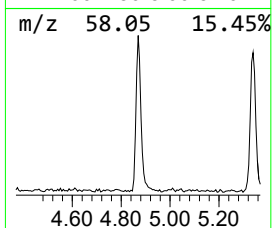
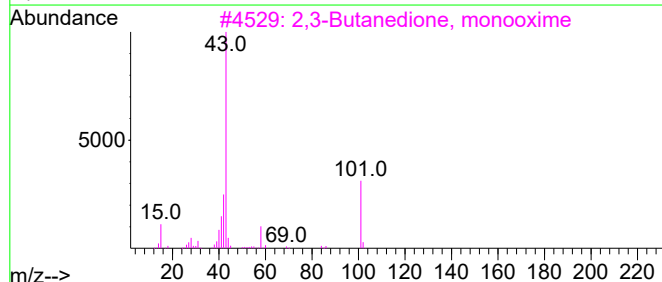
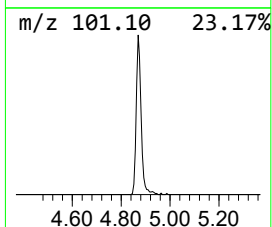
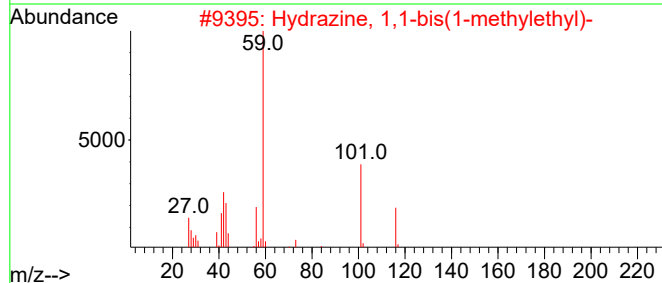
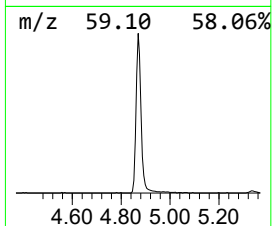
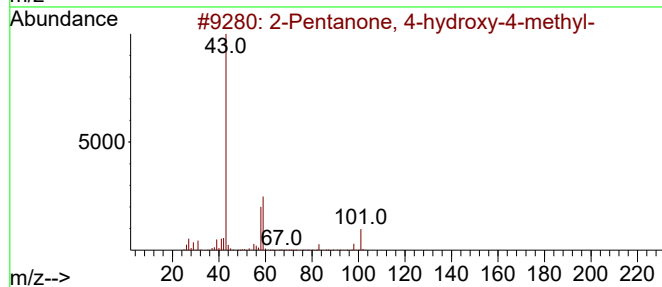
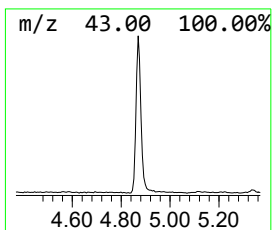
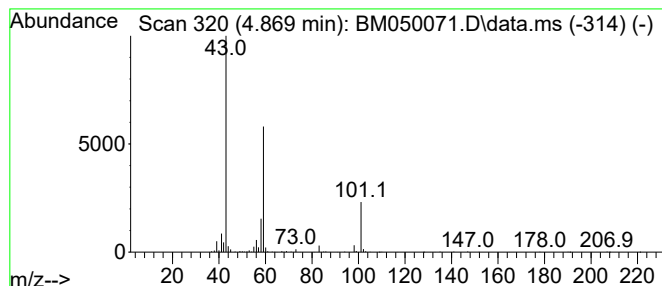
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.869	4.90 ng	369121	1,4-Dichlorobenzene-d4	7.745

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
4	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25		
5	Tetraglyme	222	C10H22O5	000143-24-8	25		



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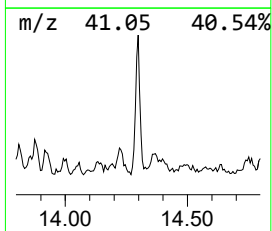
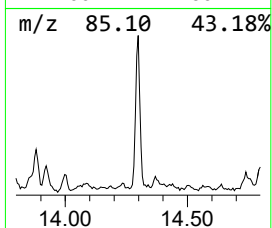
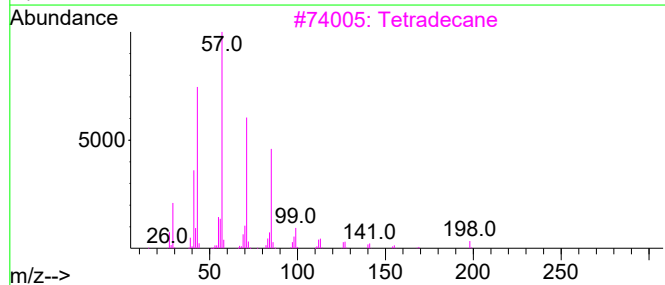
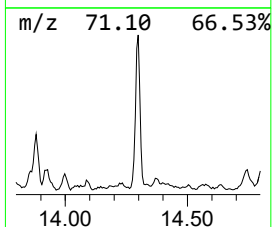
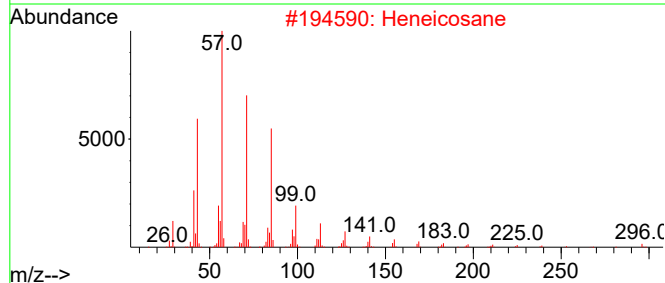
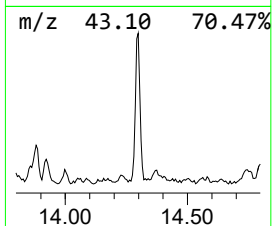
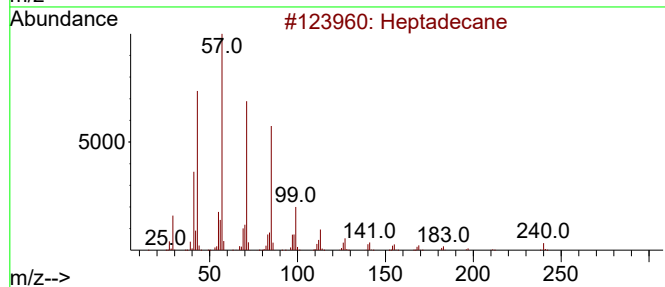
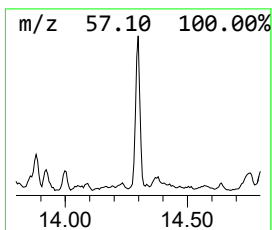
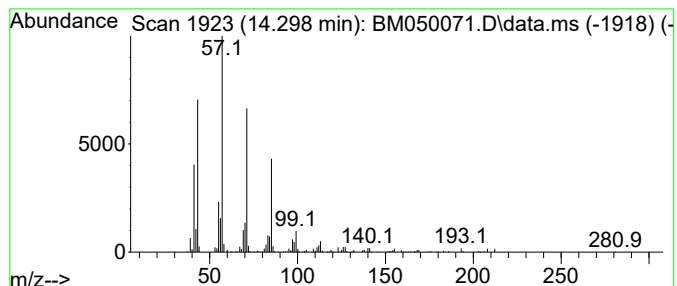
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.298	2.23 ng	318429	Acenaphthene-d10	14.392

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Tetradecane	198	C14H30	000629-59-4	87
4		Dodecane, 2-methyl-	184	C13H28	001560-97-0	86
5		9-methylheptadecane	254	C18H38	026741-18-4	86



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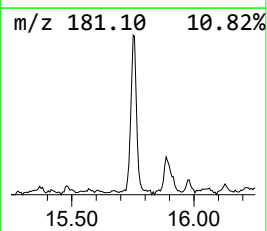
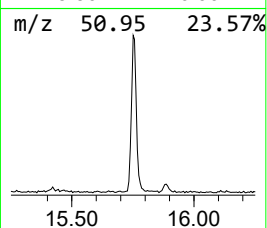
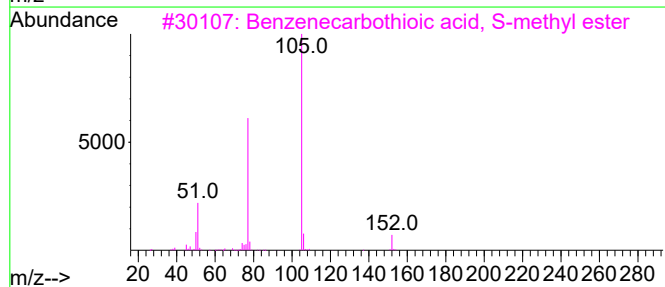
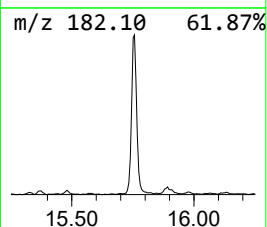
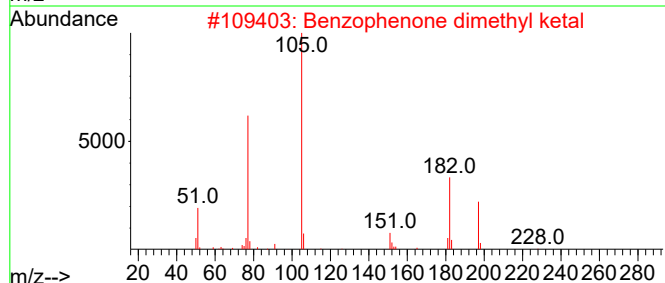
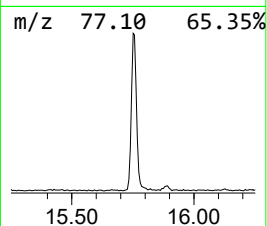
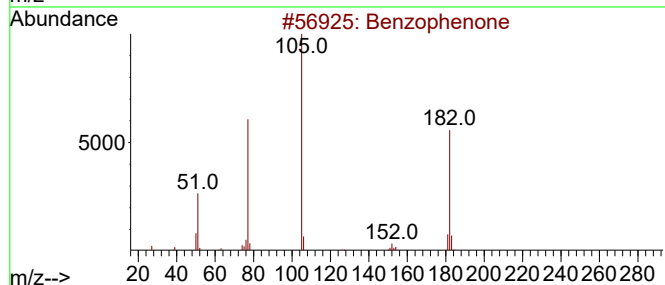
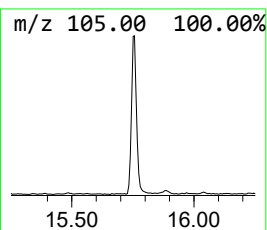
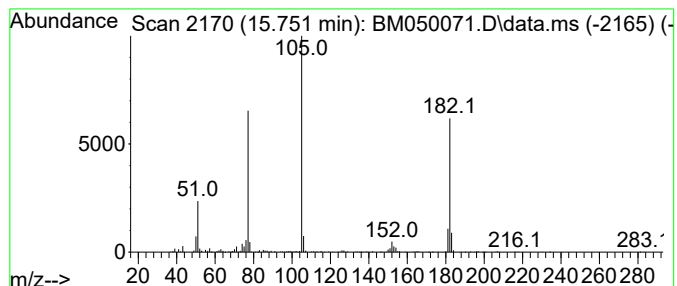
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.751	4.46 ng	638320	Acenaphthene-d10	14.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzophenone dimethyl ketal	228	C15H16O2	002235-01-0	72
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
4			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
5			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47



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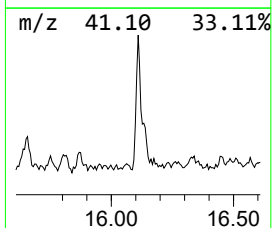
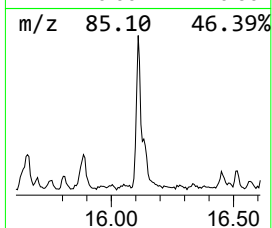
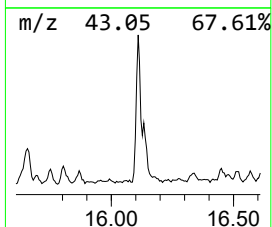
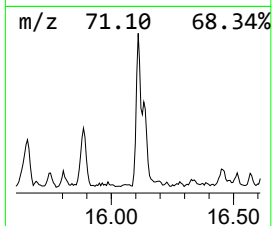
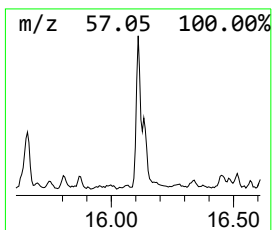
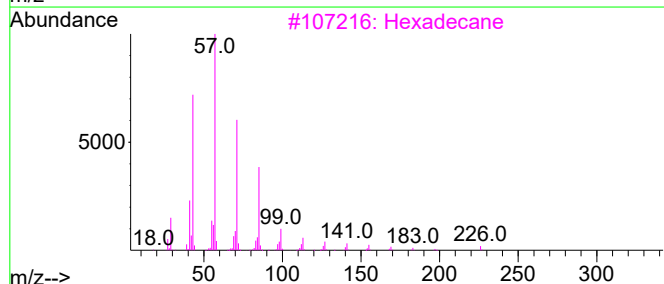
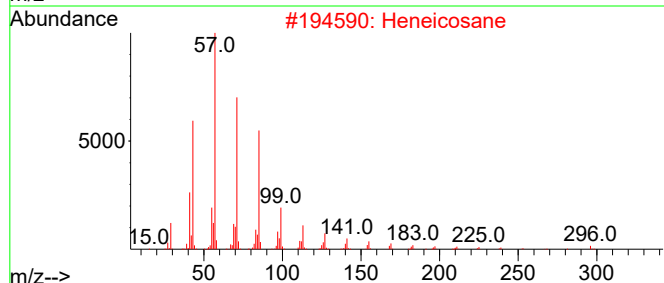
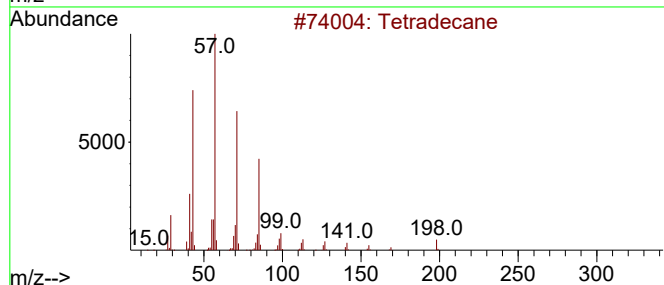
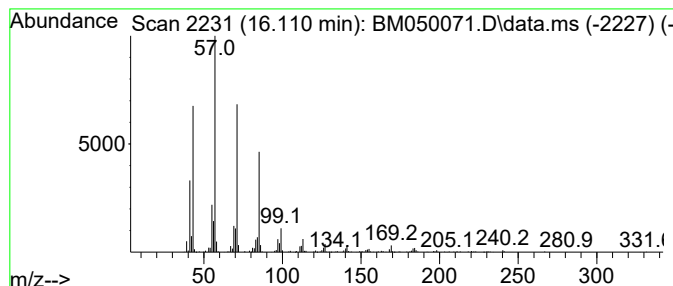
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.110	2.20 ng	367722	Phenanthrene-d10	17.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	95
2			Heneicosane	296	C21H44	000629-94-7	91
3			Hexadecane	226	C16H34	000544-76-3	91
4			Pentadecane	212	C15H32	000629-62-9	91
5			Heptadecane	240	C17H36	000629-78-7	90



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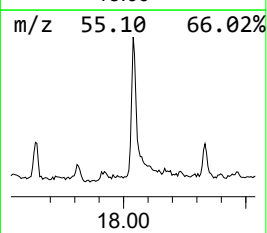
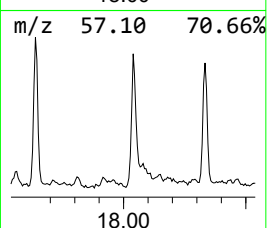
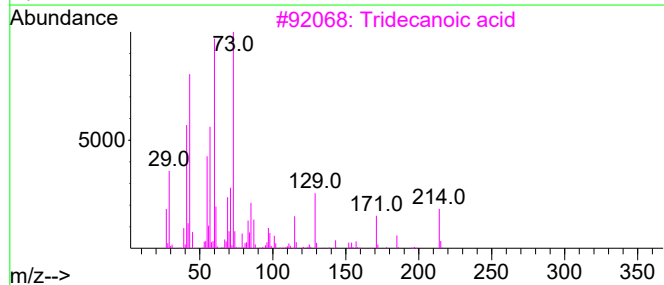
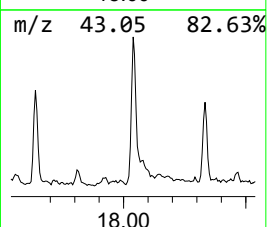
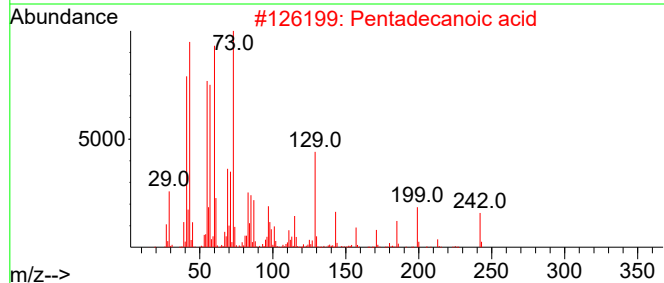
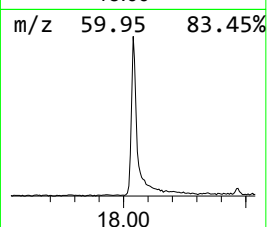
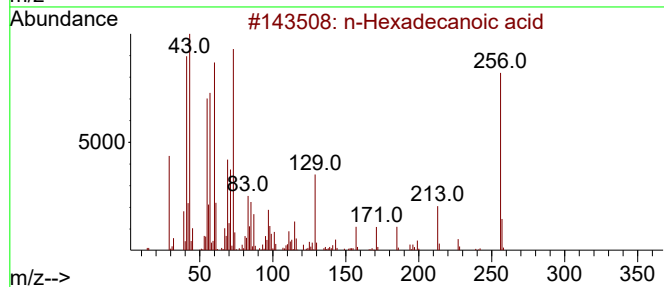
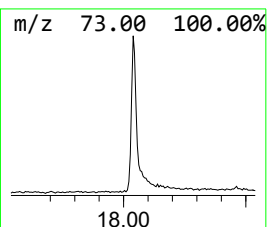
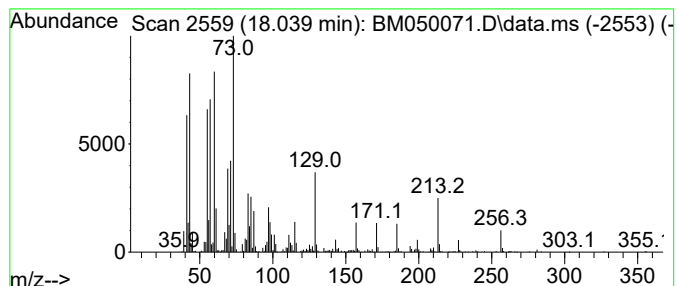
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.039	6.13 ng	1025350	Phenanthrene-d10	17.139

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	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	89
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM050125\
Data File : BM050071.D
Acq On : 01 May 2025 19:20
Operator : RC/JU
Sample : Q1914-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

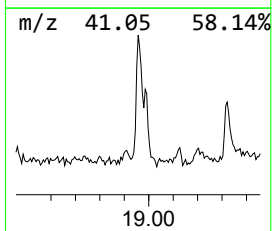
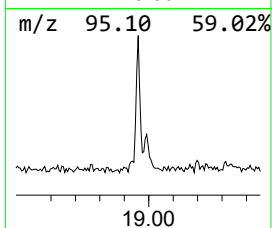
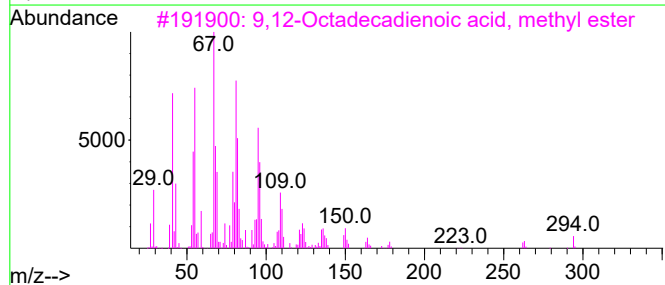
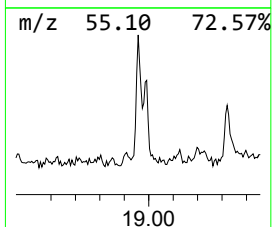
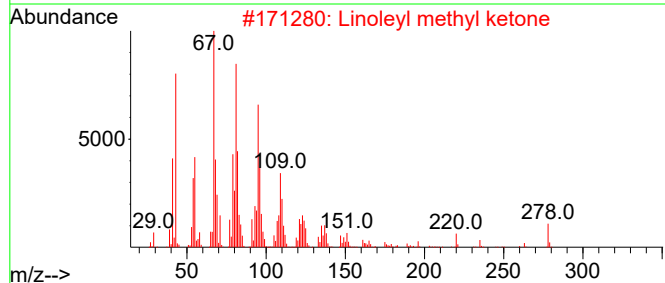
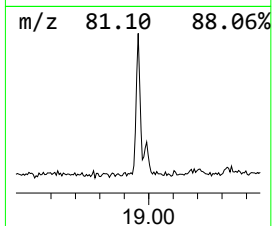
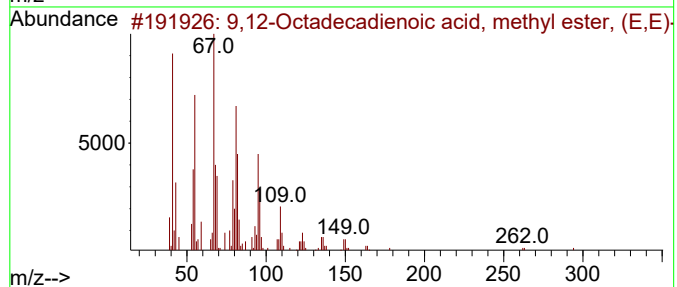
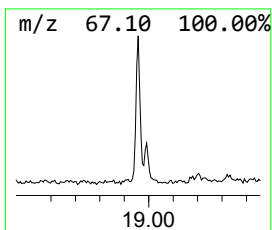
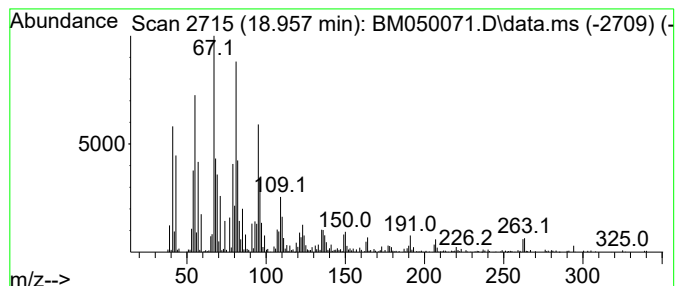
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.956	3.43 ng	573991	Phenanthrene-d10	17.139	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	Linoleyl methyl ketone	278	C19H34O	029204-24-8	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
4	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99
5	9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	98



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM050125\
Data File : BM050071.D
Acq On : 01 May 2025 19:20
Operator : RC/JU
Sample : Q1914-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SS-2

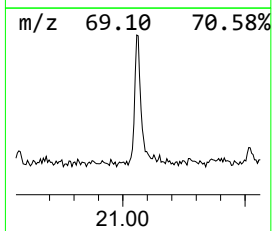
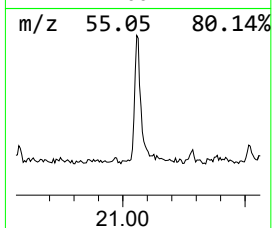
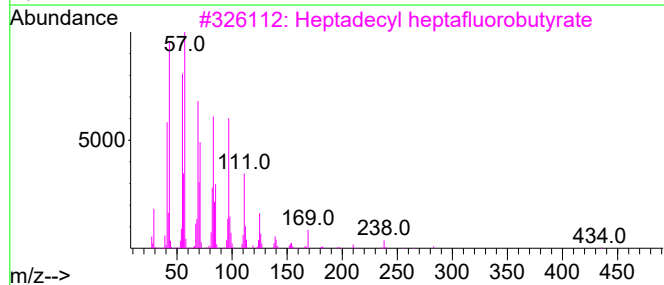
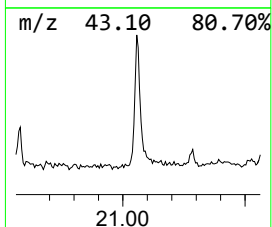
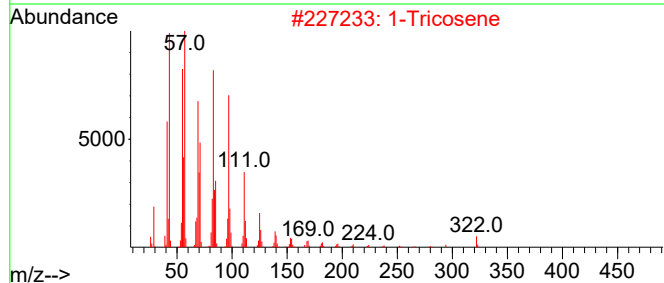
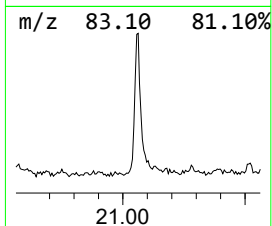
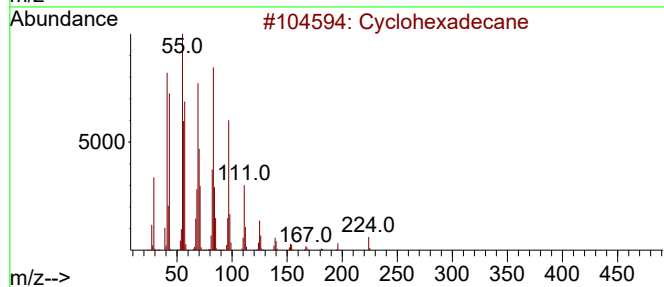
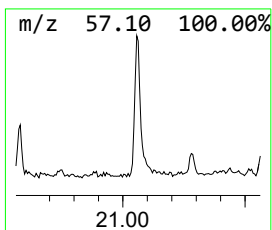
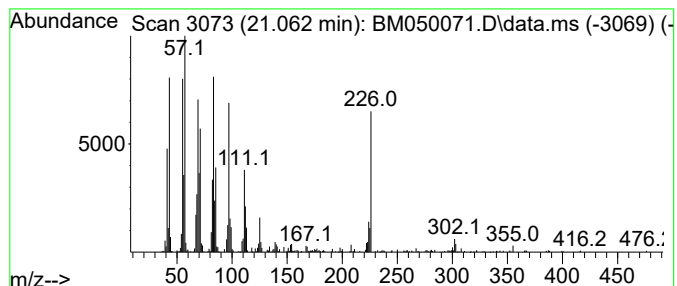
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclohexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.062	2.15 ng	491504	Chrysene-d12	21.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	98
2			1-Tricosene	322	C23H46	018835-32-0	83
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	81
4			Hexadecyl propyl ether	284	C19H40O	1000406-27-9	81
5			1-Heptacosanol	396	C27H56O	002004-39-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM050125\
Data File : BM050071.D
Acq On : 01 May 2025 19:20
Operator : RC/JU
Sample : Q1914-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SS-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.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-...	4.869	4.9	ng	369121	1	7.745	1506430	20.0
Heptadecane	14.298	2.2	ng	318429	3	14.392	2861400	20.0
Benzophenone	15.751	4.5	ng	638320	3	14.392	2861400	20.0
Tetradecane	16.110	2.2	ng	367722	4	17.139	3346560	20.0
n-Hexadecanoic ...	18.039	6.1	ng	1025350	4	17.139	3346560	20.0
9,12-Octadecadi...	18.956	3.4	ng	573991	4	17.139	3346560	20.0
Cyclohexadecane	21.062	2.1	ng	491504	5	21.380	4570510	20.0