

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042325\
 Data File : BM050016.D
 Acq On : 23 Apr 2025 16:35
 Operator : RC/JU
 Sample : Q1858-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 COMP-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-BM040825.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM050016.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.881	316	322	331	rBV	828641	1158129	10.94%	1.664%
2	5.352	396	402	420	rBV	3167819	4911541	46.41%	7.056%
3	5.957	500	505	513	rBV	155267	228704	2.16%	0.329%
4	6.946	662	673	694	rBV	2690864	4857706	45.90%	6.978%
5	7.763	804	812	822	rBV	954665	1515943	14.32%	2.178%
6	8.922	999	1009	1029	rBV	1717326	3055989	28.88%	4.390%
7	10.557	1279	1287	1301	rBV	1060387	1941419	18.35%	2.789%
8	13.028	1700	1707	1726	rBV	4690632	7116405	67.25%	10.223%
9	14.410	1936	1942	1949	rBV	1629335	2522795	23.84%	3.624%
10	15.233	2071	2082	2085	rBV	57676	126803	1.20%	0.182%
11	15.769	2166	2173	2188	rBV	1026768	1576201	14.89%	2.264%
12	15.904	2189	2196	2216	rVV	3654995	5601030	52.93%	8.046%
13	16.333	2264	2269	2275	rBV	156248	224534	2.12%	0.323%
14	17.157	2403	2409	2413	rBV	2076174	3003653	28.38%	4.315%
15	17.198	2413	2416	2423	rVV	603670	847457	8.01%	1.217%
16	17.292	2427	2432	2438	rVB	107539	169409	1.60%	0.243%
17	17.568	2470	2479	2490	rBV2	67720	220784	2.09%	0.317%
18	18.057	2553	2562	2565	rBV	568324	1015805	9.60%	1.459%
19	18.121	2570	2573	2578	rVB	78344	119665	1.13%	0.172%
20	18.227	2586	2591	2595	rBV2	108902	206862	1.95%	0.297%
21	18.480	2630	2634	2637	rBV2	115905	154487	1.46%	0.222%
22	18.586	2648	2652	2660	rVB3	55428	112151	1.06%	0.161%
23	18.951	2710	2714	2717	rBV	76851	108854	1.03%	0.156%
24	19.215	2754	2759	2763	rBV	1227546	1604967	15.17%	2.306%
25	19.257	2763	2766	2774	rVV3	277690	632082	5.97%	0.908%
26	19.333	2775	2779	2789	rVB3	342279	603558	5.70%	0.867%
27	19.580	2812	2821	2830	rBV	986764	1596972	15.09%	2.294%
28	19.780	2849	2855	2861	rBV	9691619	10582764	100.00%	15.202%
29	21.074	3071	3075	3084	rVB3	257430	468470	4.43%	0.673%
30	21.398	3123	3130	3134	rBV2	2657485	4384734	41.43%	6.299%
31	21.439	3134	3137	3148	rVB	507302	775931	7.33%	1.115%
32	22.498	3312	3317	3329	rVB	848953	1382572	13.06%	1.986%
33	22.774	3359	3364	3377	rVB	1021428	1860237	17.58%	2.672%
34	23.450	3475	3479	3486	rBV	302902	696883	6.59%	1.001%
35	24.256	3612	3616	3627	rVB	303517	665693	6.29%	0.956%
36	24.397	3632	3640	3649	rBV	1434802	3561263	33.65%	5.116%

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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-BM040825.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

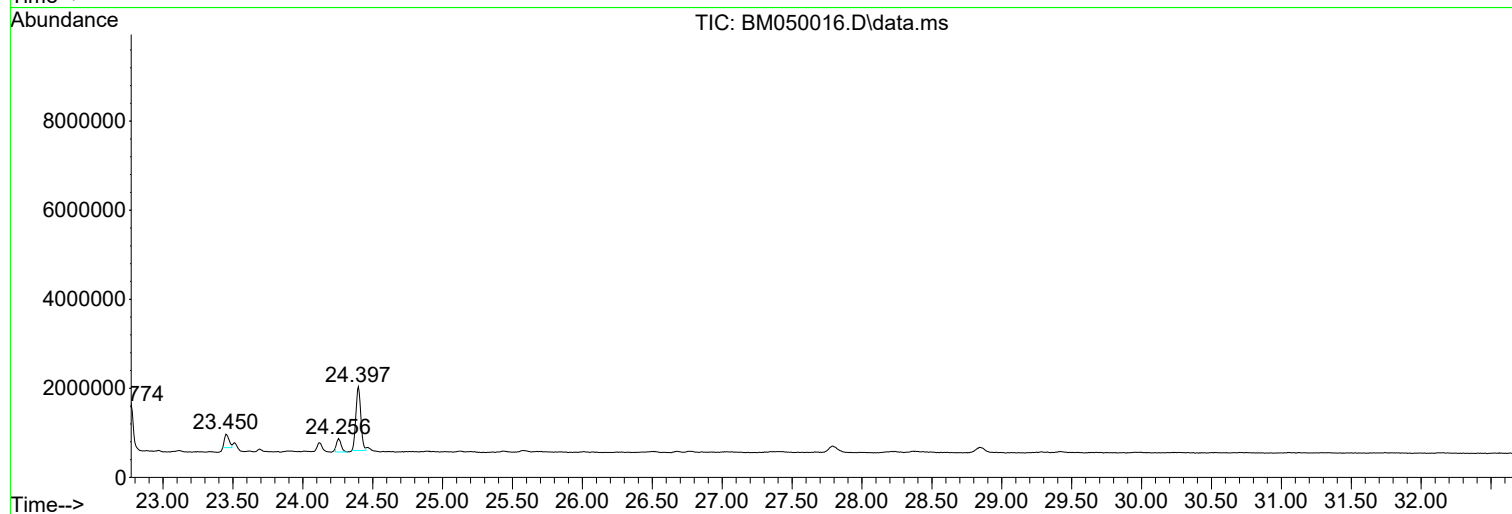
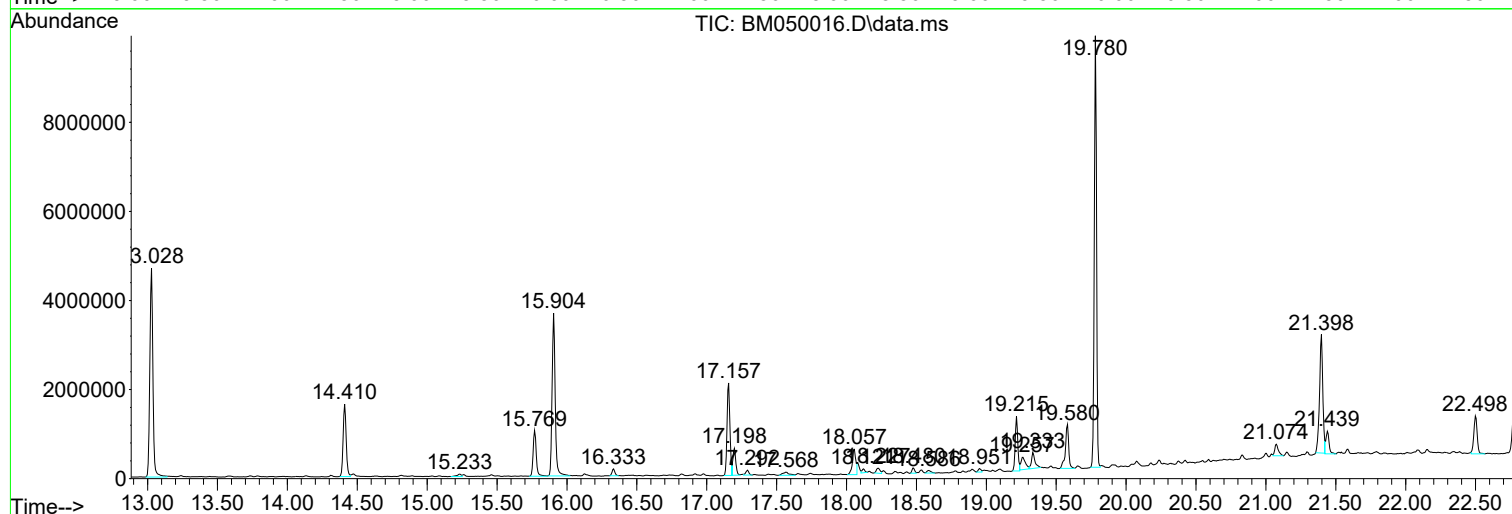
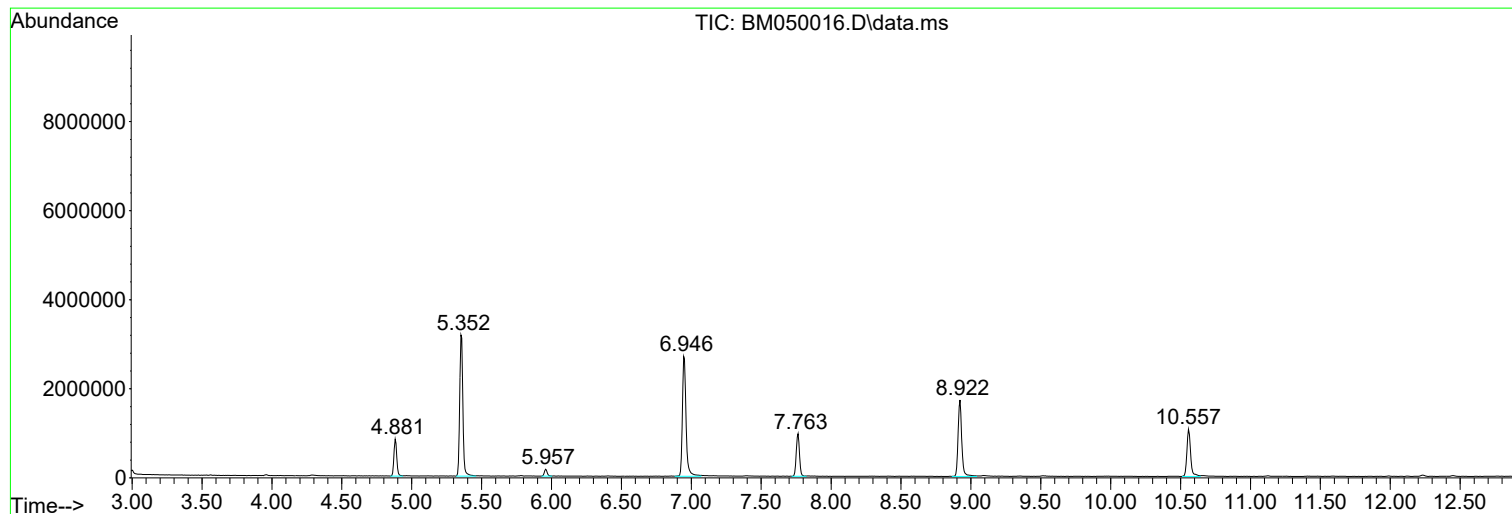
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BM050016.D
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Operator : RC/JU
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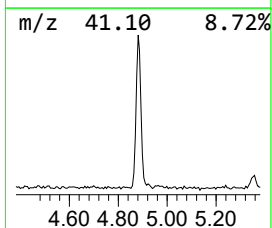
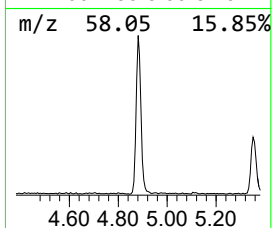
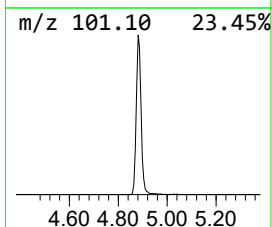
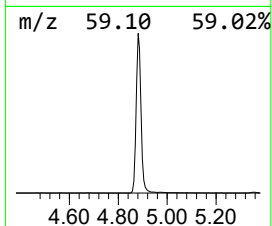
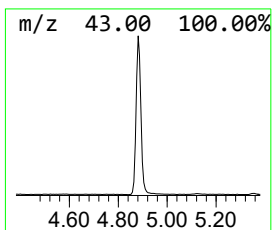
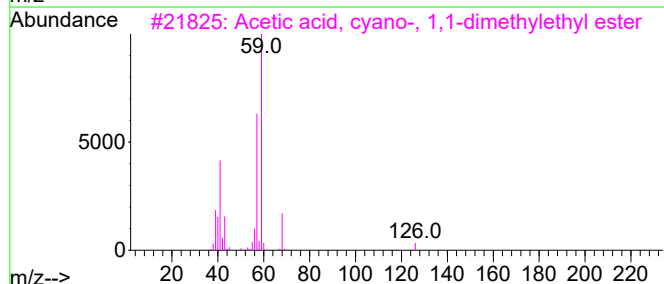
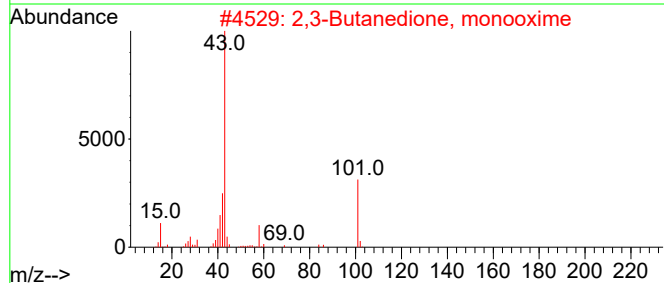
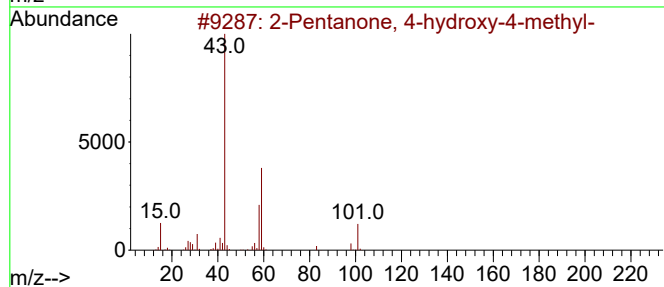
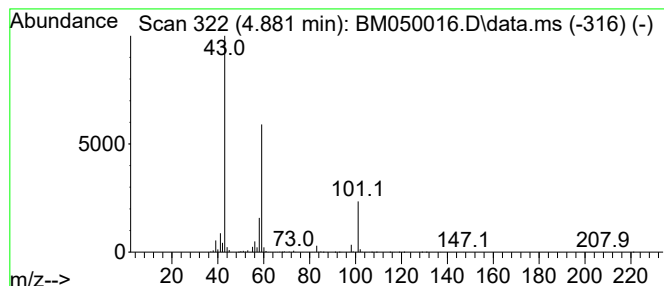
Instrument :
BNA_M
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.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 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.881	15.28 ng	1158130	1,4-Dichlorobenzene-d4	7.763	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9



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Misc :
ALS Vial : 11 Sample Multiplier: 1

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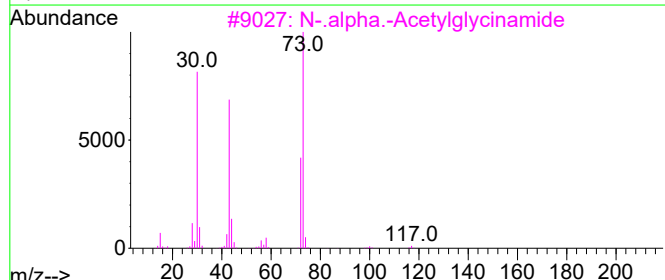
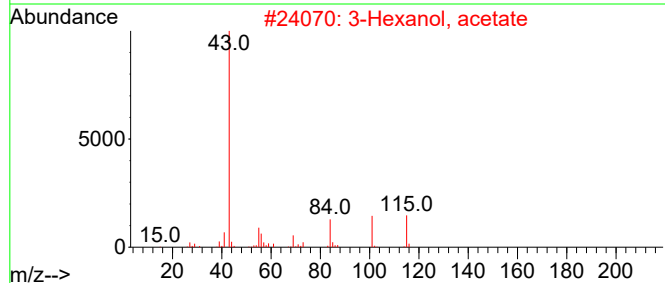
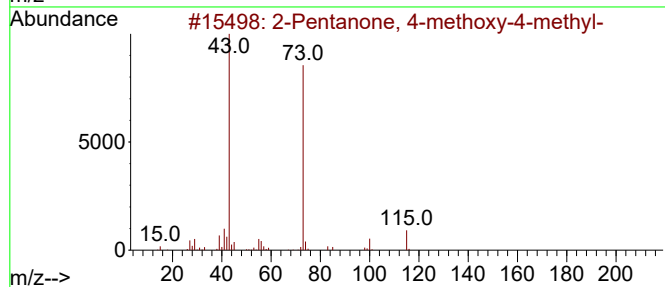
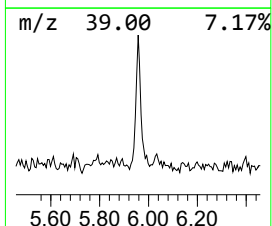
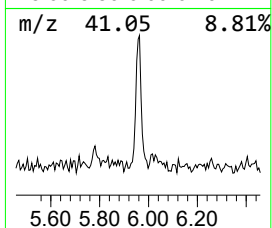
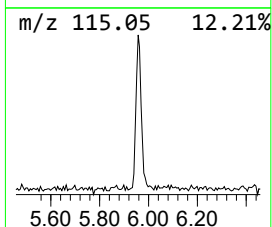
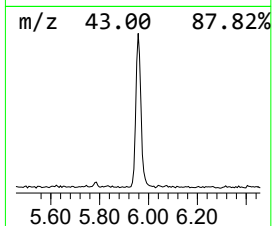
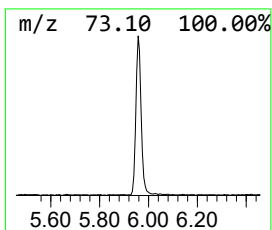
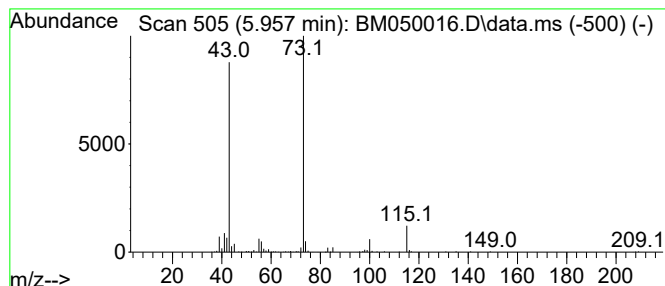
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.957	3.02 ng	228704	1,4-Dichlorobenzene-d4	7.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		3-Hexanol, acetate	144	C8H16O2	040780-64-1	32
3		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	28
4		3-Heptanol, 3,5-dimethyl-	144	C9H20O	019549-74-7	25
5		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	22



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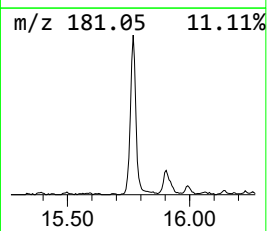
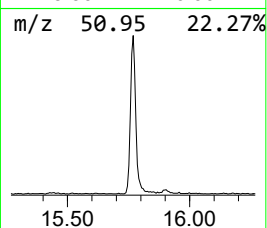
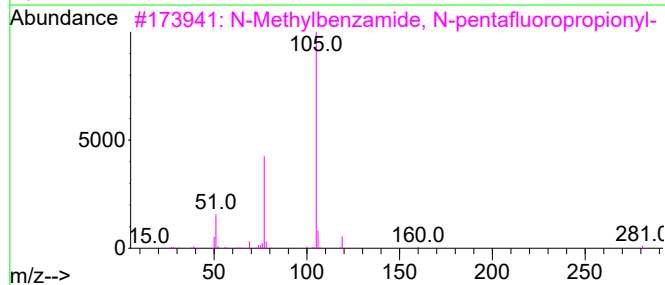
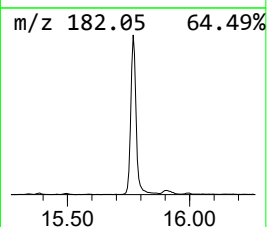
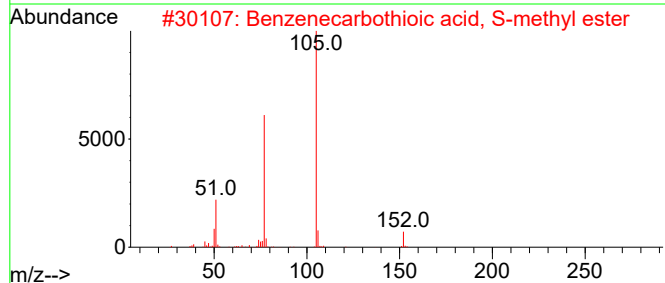
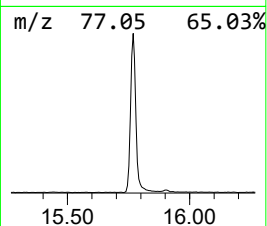
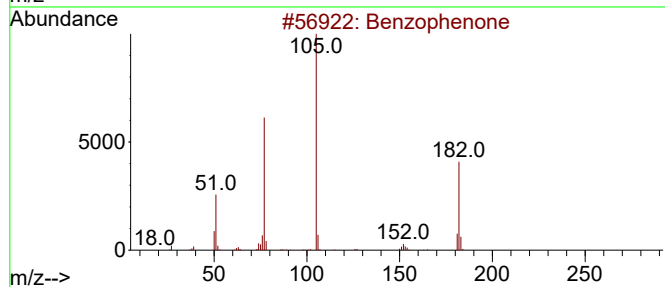
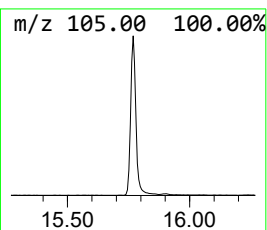
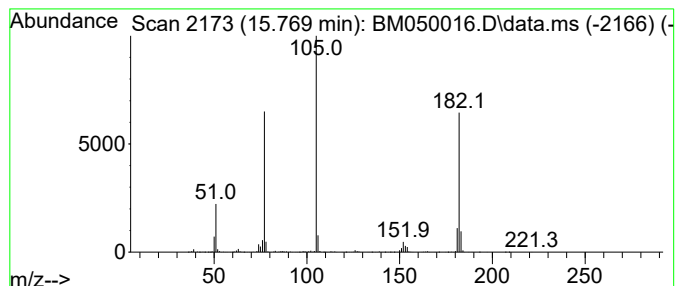
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.769	12.50 ng	1576200	Acenaphthene-d10	14.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
3			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	43
4			Benzenecarbothioic acid	138	C7H6OS	000098-91-9	43
5			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	43



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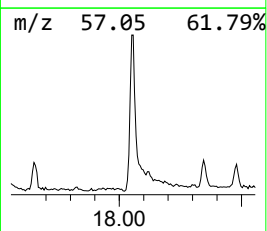
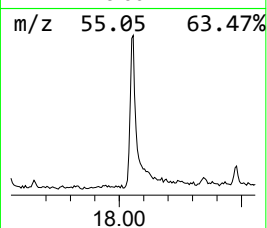
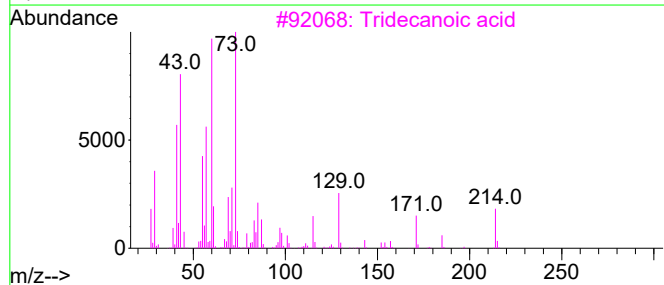
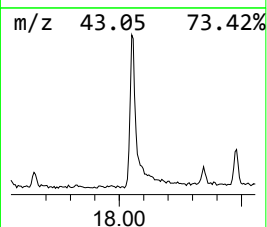
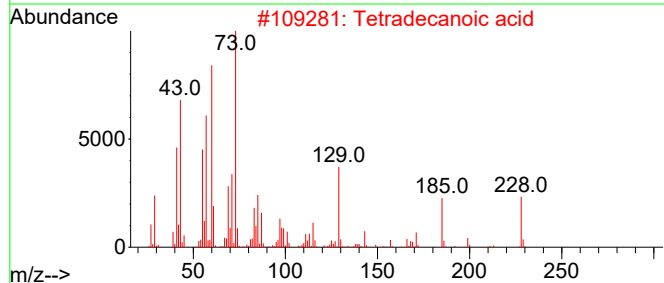
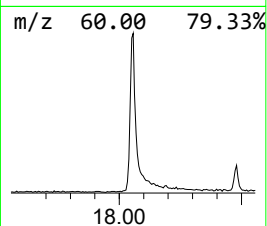
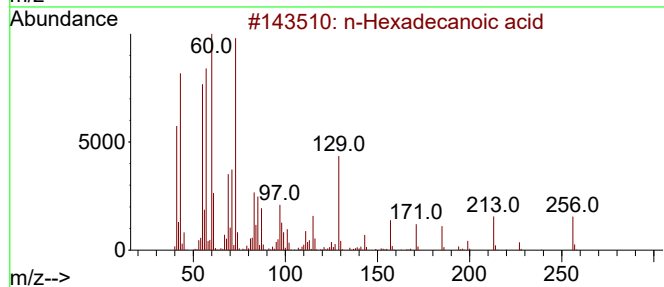
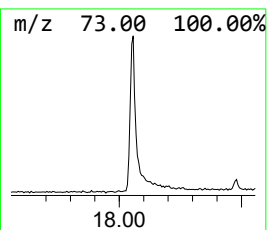
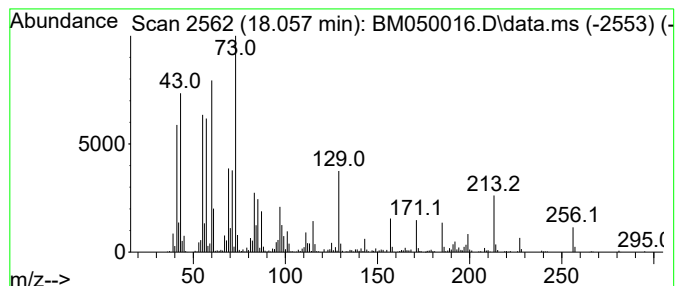
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.057	6.76 ng	1015810	Phenanthrene-d10	17.157

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	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Octadecanoic acid	284	C18H36O2	000057-11-4	81



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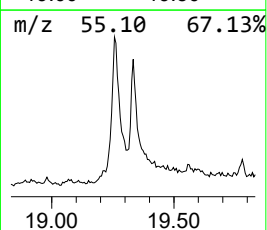
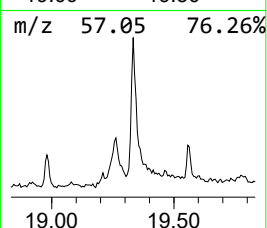
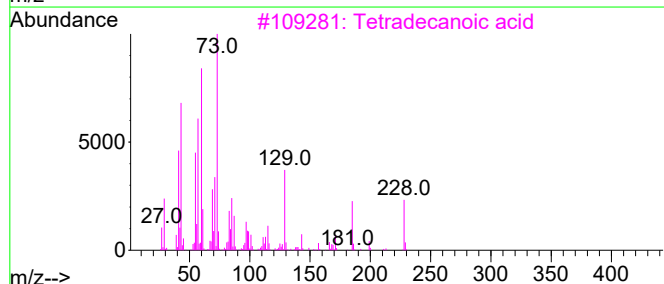
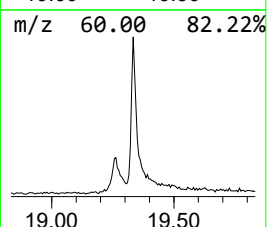
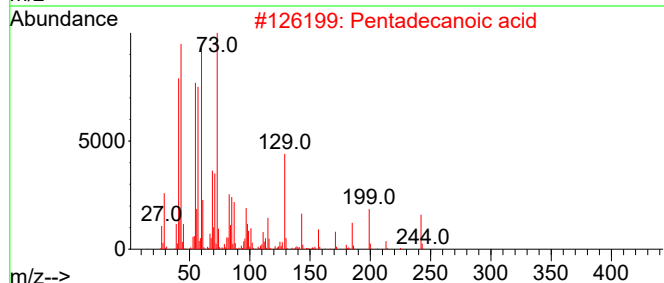
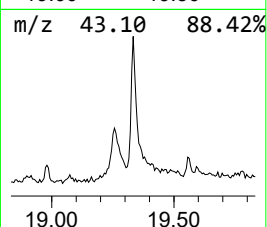
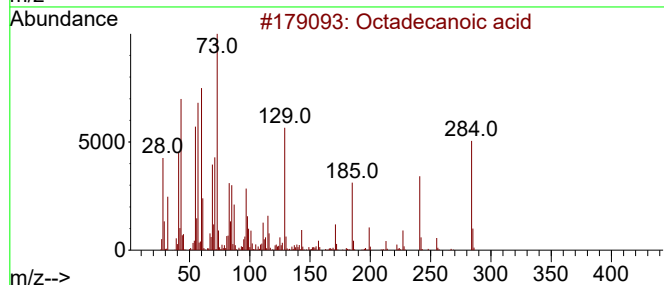
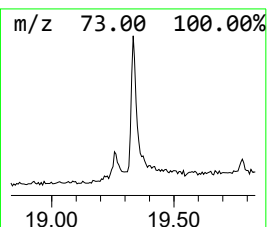
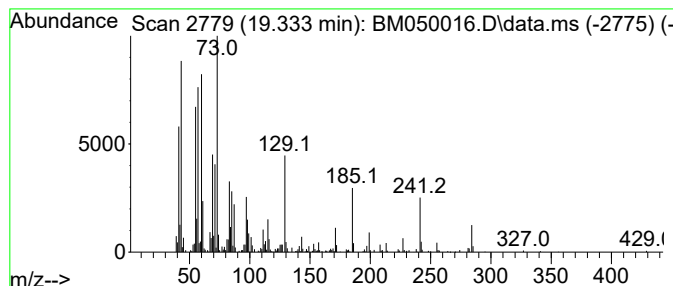
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.333	2.75 ng	603558	Chrysene-d12	21.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042325\
Data File : BM050016.D
Acq On : 23 Apr 2025 16:35
Operator : RC/JU
Sample : Q1858-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
COMP-2

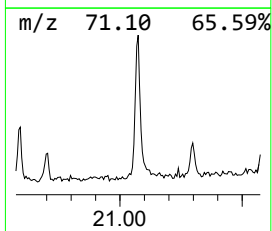
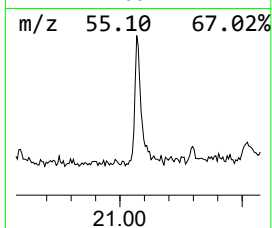
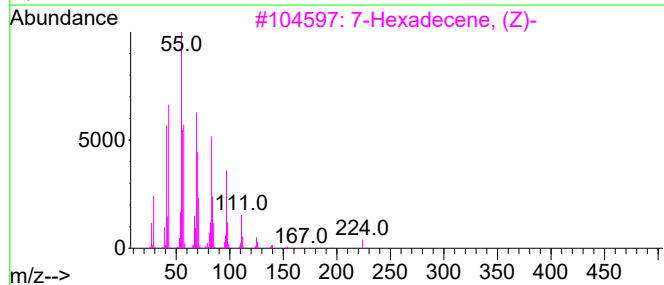
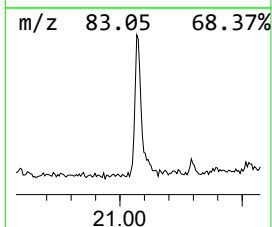
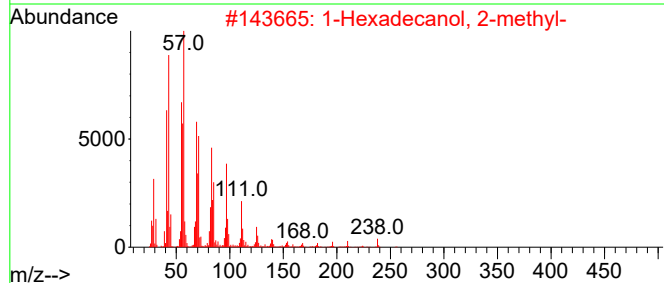
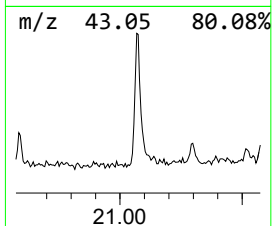
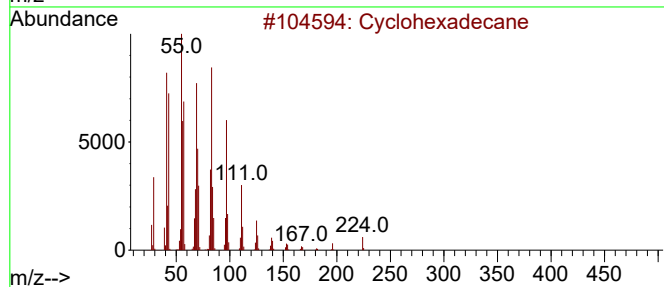
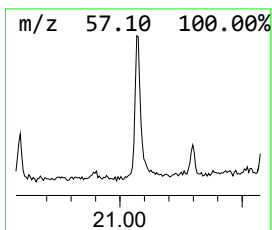
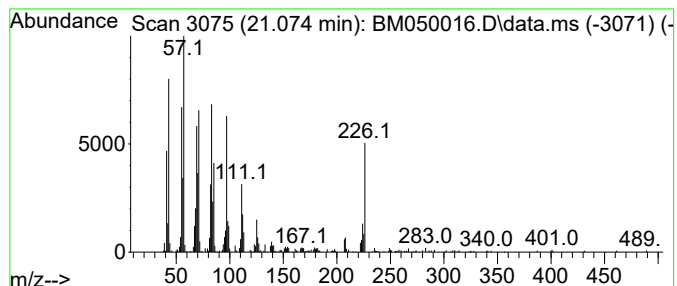
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclohexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.074	2.14 ng	468470	Chrysene-d12	21.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	95
2			1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	93
3			7-Hexadecene, (Z)-	224	C16H32	035507-09-6	90
4			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	89
5			Hexadecyl propyl ether	284	C19H40O	1000406-27-9	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042325\
Data File : BM050016.D
Acq On : 23 Apr 2025 16:35
Operator : RC/JU
Sample : Q1858-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-2

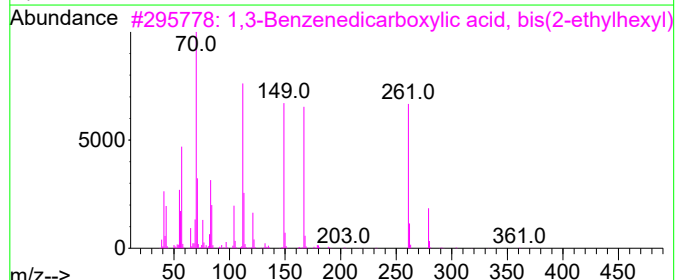
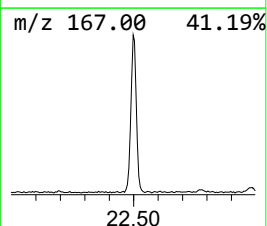
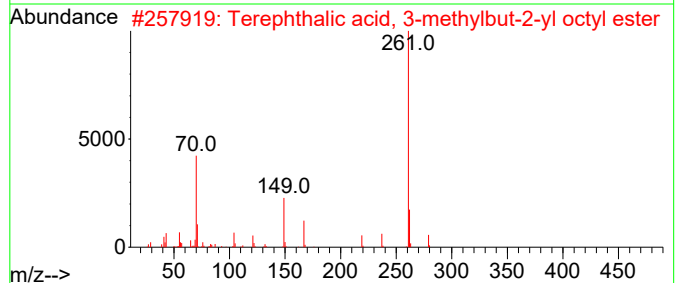
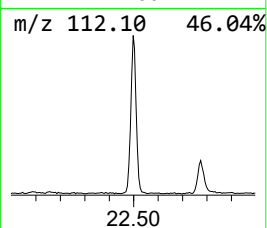
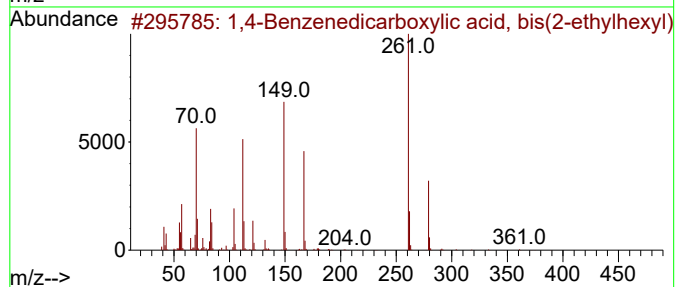
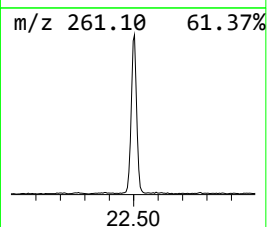
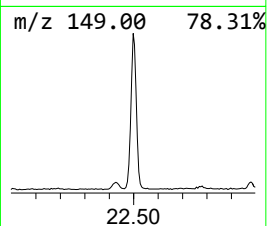
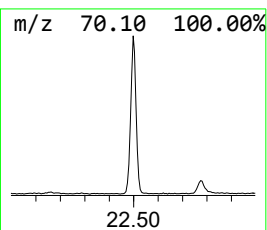
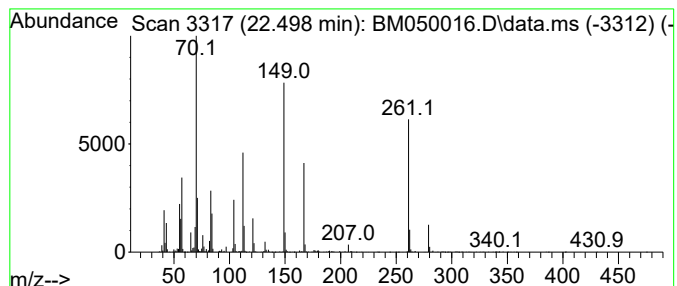
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,4-Benzenedicarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.497	6.31 ng	1382570	Chrysene-d12	21.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	87
2			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	72
3			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	47
4			Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	46
5			Phthalic acid, 6-ethyloct-3-yl 2...	418	C26H42O4	1000315-53-8	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042325\
Data File : BM050016.D
Acq On : 23 Apr 2025 16:35
Operator : RC/JU
Sample : Q1858-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-2

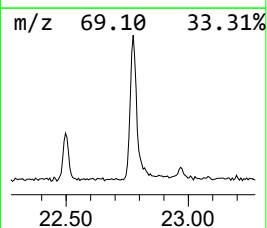
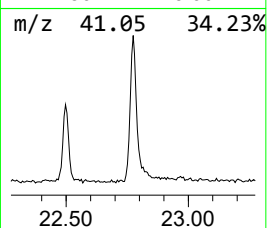
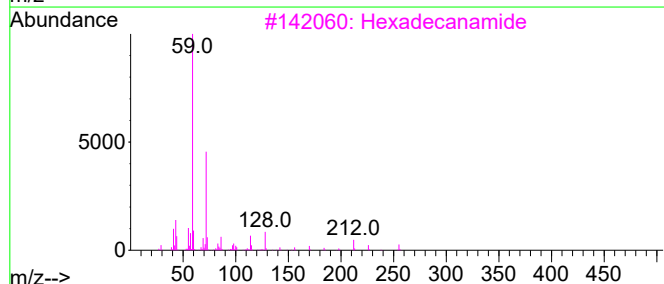
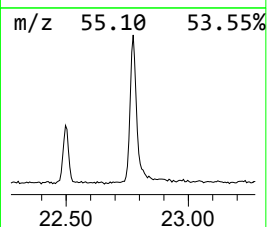
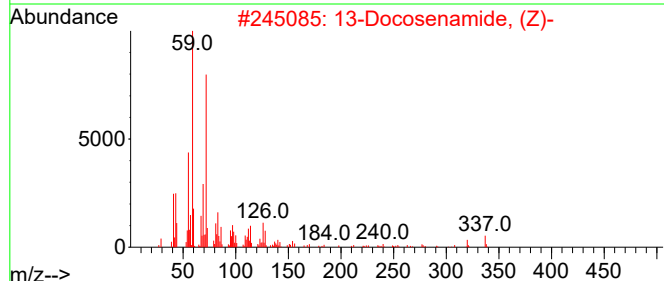
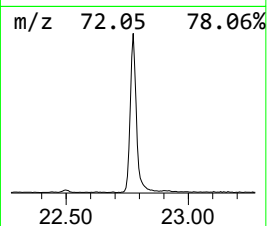
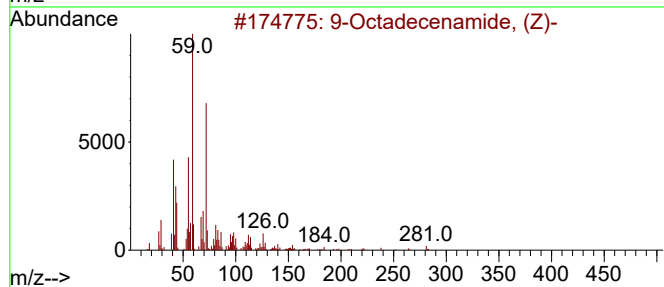
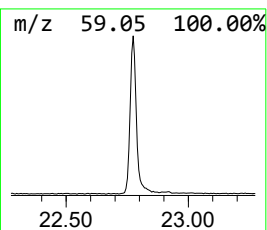
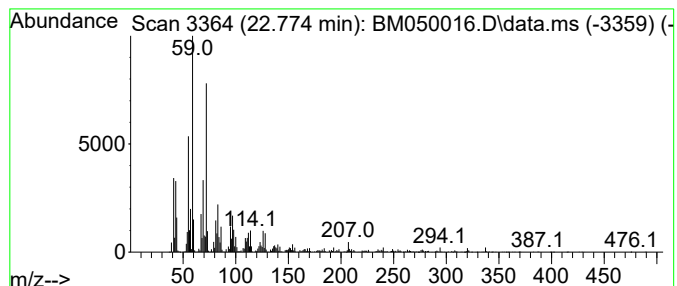
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.774	8.49 ng	1860240	Chrysene-d12	21.398

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	86
3		Hexadecanamide	255	C16H33NO	000629-54-9	59
4		Palmitoleamide	253	C16H31NO	106010-22-4	59
5		Octadecanamide	283	C18H37NO	000124-26-5	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042325\
Data File : BM050016.D
Acq On : 23 Apr 2025 16:35
Operator : RC/JU
Sample : Q1858-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.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
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2-Pentanone, 4-...	5.957	3.0	ng	228704	1	7.763	1515940	20.0
Benzophenone	15.769	12.5	ng	1576200	3	14.410	2522800	20.0
n-Hexadecanoic ...	18.057	6.8	ng	1015810	4	17.157	3003650	20.0
Octadecanoic acid	19.333	2.8	ng	603558	5	21.398	4384730	20.0
Cyclohexadecane	21.074	2.1	ng	468470	5	21.398	4384730	20.0
1,4-Benzenedica...	22.497	6.3	ng	1382570	5	21.398	4384730	20.0
9-Octadecenamid...	22.774	8.5	ng	1860240	5	21.398	4384730	20.0