

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042125\
 Data File : BM049988.D
 Acq On : 21 Apr 2025 17:11
 Operator : RC/JU
 Sample : Q1842-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PL-714-COMP-08

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: BM049988.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.887	317	323	334	rBV	993124	1403064	8.73%	1.328%
2	5.357	396	403	414	rBV	3839644	5837043	36.34%	5.523%
3	5.963	498	506	515	rBV	152232	239441	1.49%	0.227%
4	6.951	666	674	695	rBV	3992404	6782750	42.22%	6.418%
5	7.763	805	812	822	rBV	1523146	2356800	14.67%	2.230%
6	8.922	1001	1009	1025	rBV	2490120	4096166	25.50%	3.876%
7	10.557	1279	1287	1300	rBV	1795795	3138728	19.54%	2.970%
8	13.027	1700	1707	1724	rBV	7383186	10742526	66.87%	10.165%
9	14.410	1934	1942	1949	rBV	2973563	4452811	27.72%	4.214%
10	15.768	2166	2173	2187	rBV	1811196	2510104	15.63%	2.375%
11	15.904	2189	2196	2215	rVV	6583686	9467060	58.93%	8.958%
12	16.333	2263	2269	2275	rVB	296143	416354	2.59%	0.394%
13	17.156	2400	2409	2413	rBV	3819514	5537376	34.47%	5.240%
14	17.198	2413	2416	2422	rVB	1155088	1507208	9.38%	1.426%
15	17.292	2427	2432	2437	rVB	168891	265714	1.65%	0.251%
16	17.562	2470	2478	2491	rBV	84758	234509	1.46%	0.222%
17	18.056	2553	2562	2571	rBV2	1808549	3233939	20.13%	3.060%
18	18.227	2586	2591	2595	rBV2	287201	489476	3.05%	0.463%
19	18.262	2595	2597	2603	rVB	141442	170004	1.06%	0.161%
20	18.580	2647	2651	2661	rVB2	152611	256757	1.60%	0.243%
21	19.215	2754	2759	2766	rBV	2633987	3366216	20.96%	3.185%
22	19.333	2775	2779	2789	rBV2	478148	808542	5.03%	0.765%
23	19.456	2798	2800	2810	rVB2	101597	185084	1.15%	0.175%
24	19.580	2811	2821	2829	rVV	2253184	3611188	22.48%	3.417%
25	19.780	2849	2855	2860	rBV	13753552	16063969	100.00%	15.201%
26	19.903	2872	2876	2883	rBV3	121756	266452	1.66%	0.252%
27	20.074	2901	2905	2913	rVB2	321644	563816	3.51%	0.534%
28	20.174	2919	2922	2926	rVB	210355	224954	1.40%	0.213%
29	20.239	2930	2933	2936	rVB2	243417	300663	1.87%	0.285%
30	21.074	3072	3075	3082	rBV3	746464	1187793	7.39%	1.124%
31	21.397	3123	3130	3135	rBV2	4116490	7256225	45.17%	6.866%
32	21.444	3135	3138	3152	rVB	976385	1680718	10.46%	1.590%
33	22.162	3257	3260	3262	rBV3	209007	303869	1.89%	0.288%
34	23.456	3475	3480	3487	rBV	476293	1237538	7.70%	1.171%
35	24.256	3611	3616	3626	rBV	403234	944751	5.88%	0.894%
36	24.403	3633	3641	3650	rVB	1838806	4537826	28.25%	4.294%

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042125\
Data File : BM049988.D
Acq On : 21 Apr 2025 17:11
Operator : RC/JU
Sample : Q1842-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PL-714-COMP-08

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

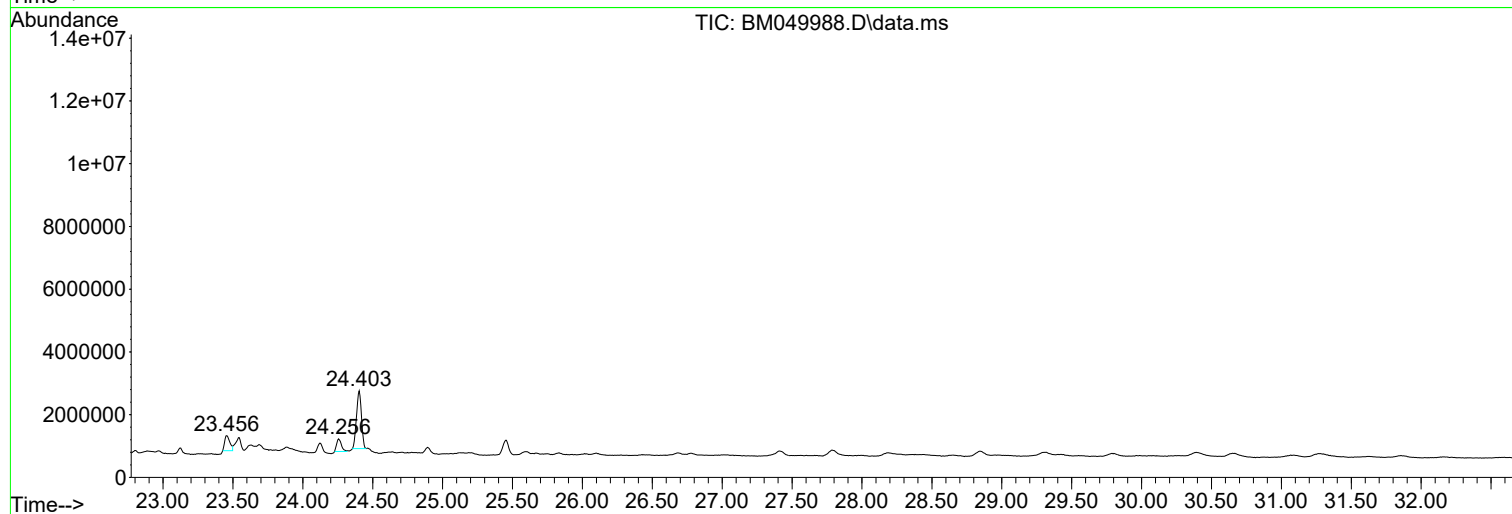
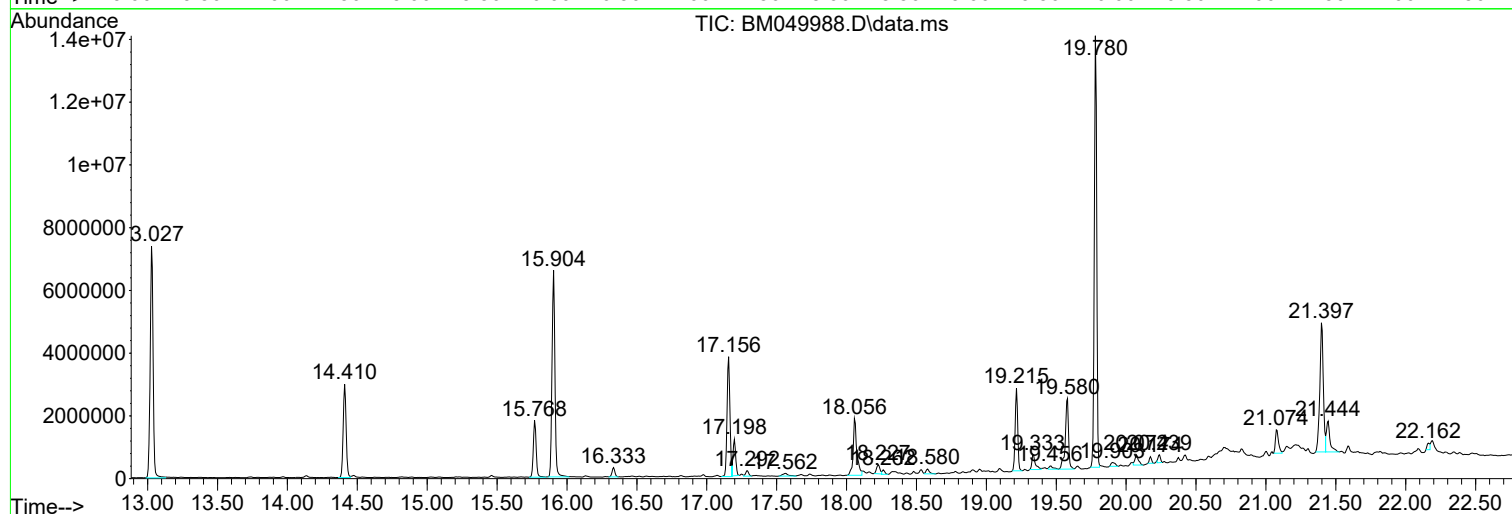
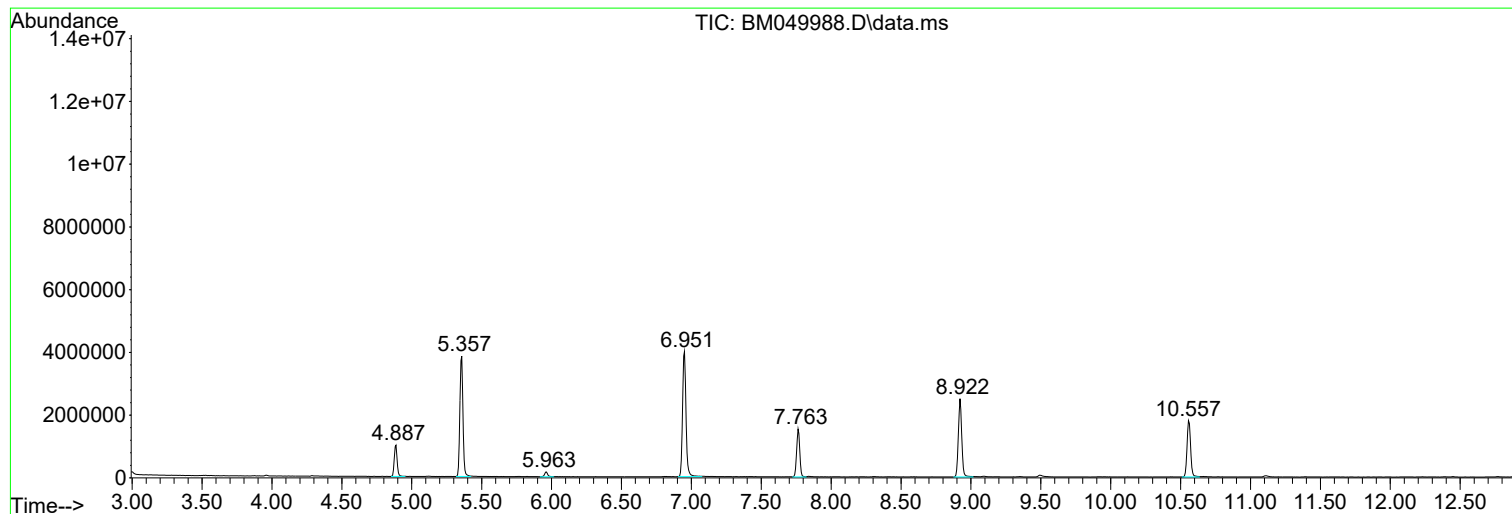
Sum of corrected areas: 105677434

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042125\
Data File : BM049988.D
Acq On : 21 Apr 2025 17:11
Operator : RC/JU
Sample : Q1842-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PL-714-COMP-08

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042125\
Data File : BM049988.D
Acq On : 21 Apr 2025 17:11
Operator : RC/JU
Sample : Q1842-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

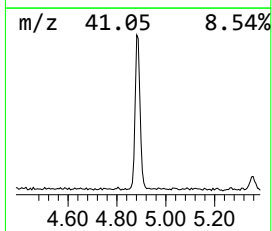
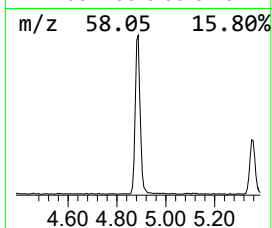
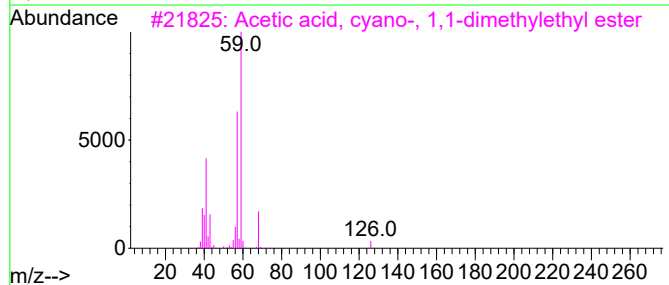
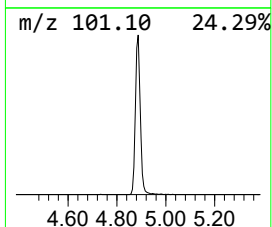
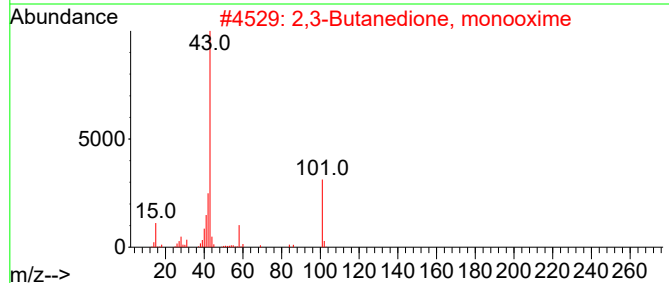
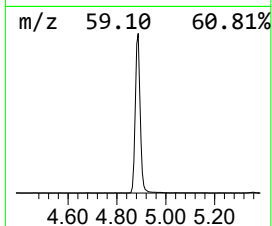
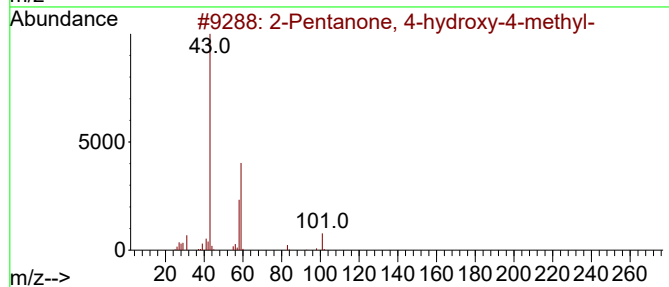
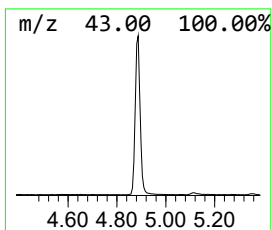
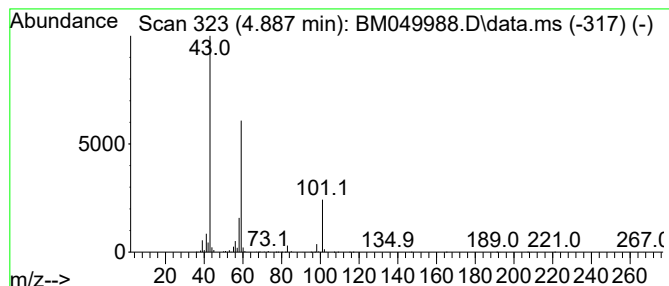
Instrument :
BNA_M
ClientSampleId :
PL-714-COMP-08

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.	
4.887	11.91 ng	1403060	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	56
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	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042125\
Data File : BM049988.D
Acq On : 21 Apr 2025 17:11
Operator : RC/JU
Sample : Q1842-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PL-714-COMP-08

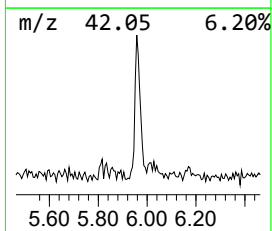
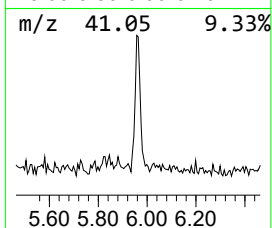
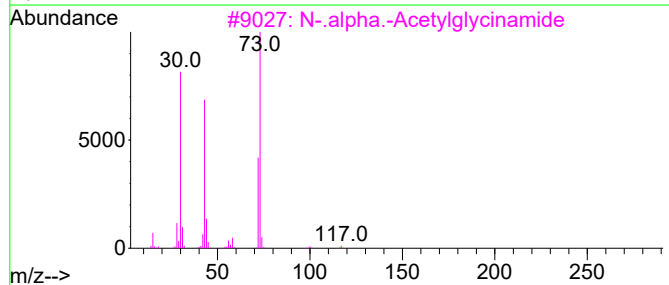
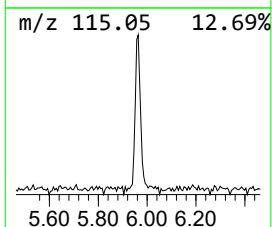
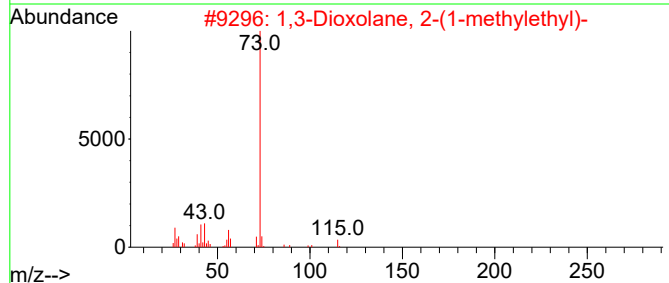
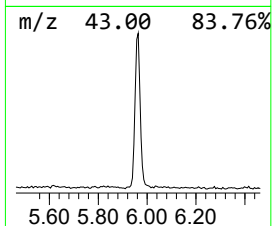
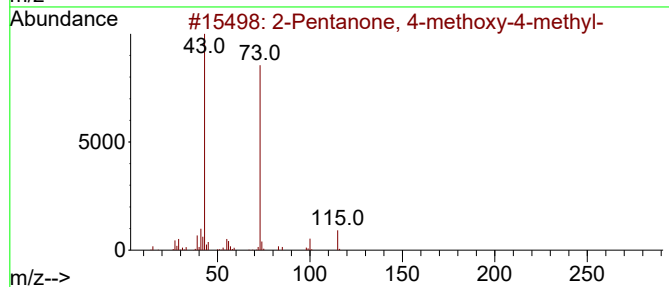
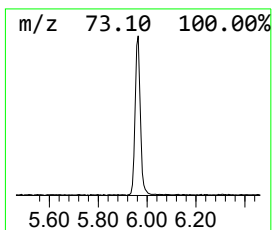
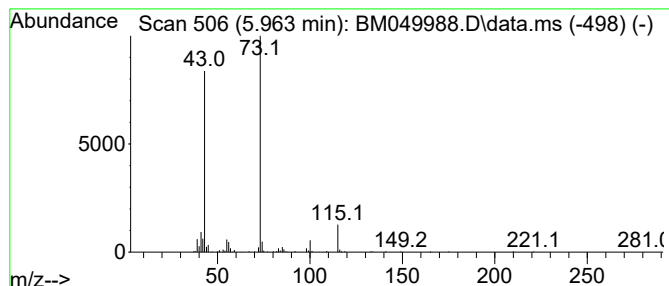
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.963	2.03 ng	239441	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	78
2		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	46
3		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	28
4		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
5		2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042125\
Data File : BM049988.D
Acq On : 21 Apr 2025 17:11
Operator : RC/JU
Sample : Q1842-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PL-714-COMP-08

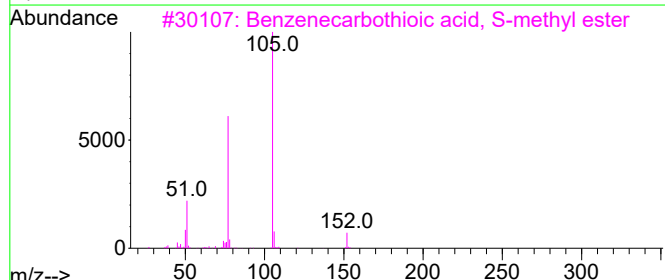
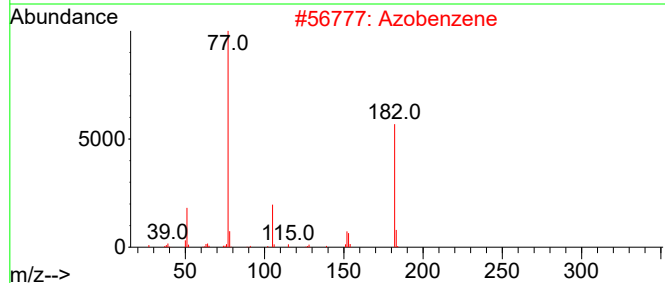
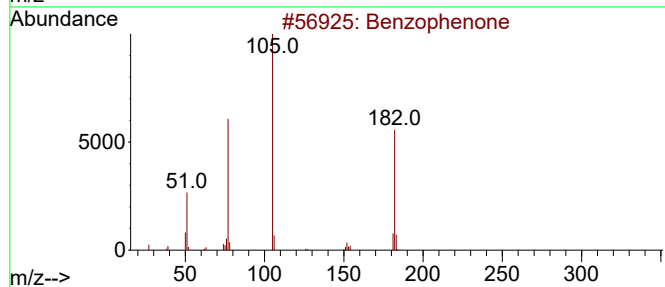
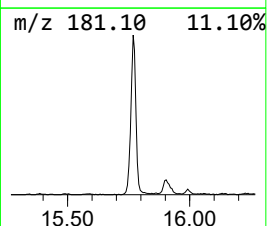
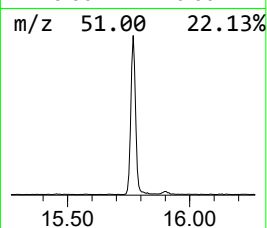
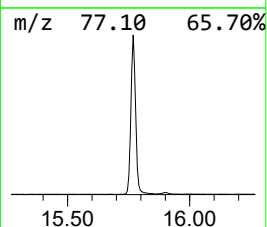
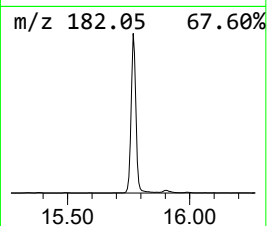
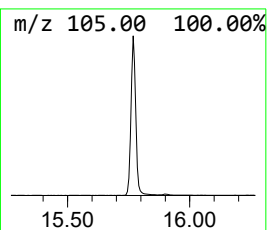
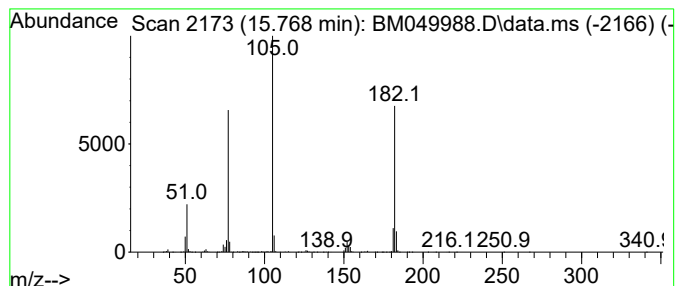
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.768	11.27 ng	2510100	Acenaphthene-d10	14.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	47
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	46
5			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042125\
Data File : BM049988.D
Acq On : 21 Apr 2025 17:11
Operator : RC/JU
Sample : Q1842-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PL-714-COMP-08

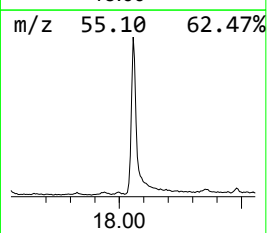
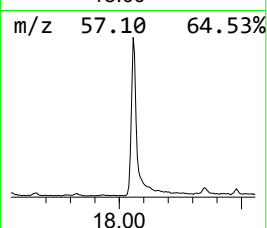
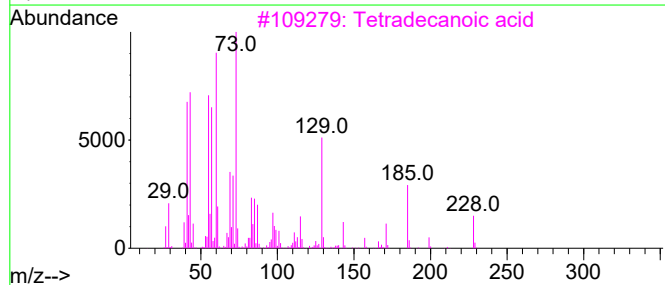
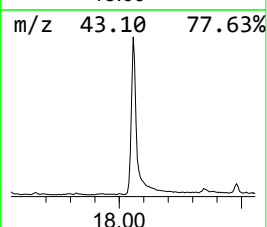
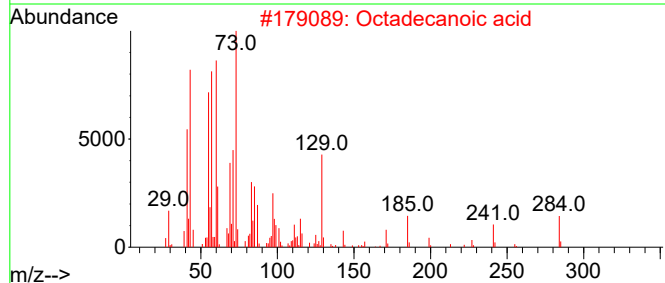
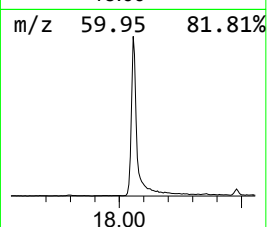
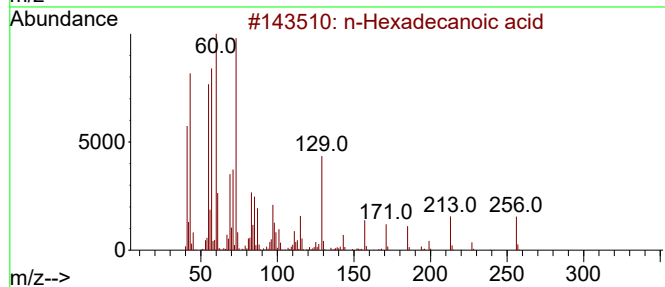
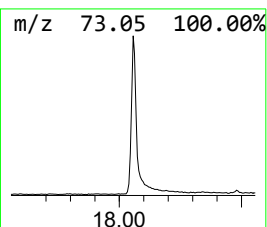
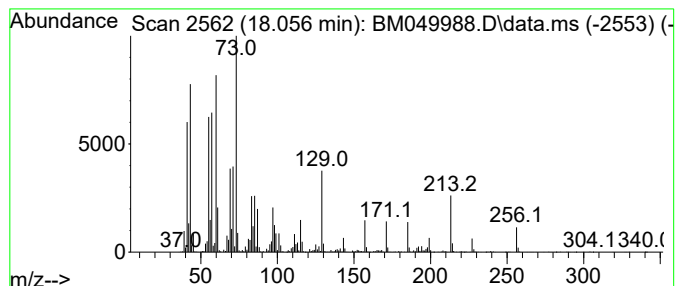
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.056	11.68 ng	3233940	Phenanthrene-d10	17.156

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			Tridecanoic acid	214	C13H26O2	000638-53-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042125\
Data File : BM049988.D
Acq On : 21 Apr 2025 17:11
Operator : RC/JU
Sample : Q1842-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PL-714-COMP-08

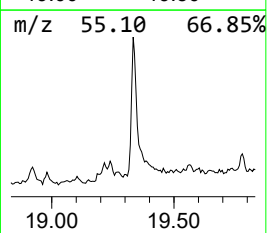
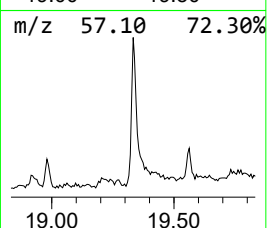
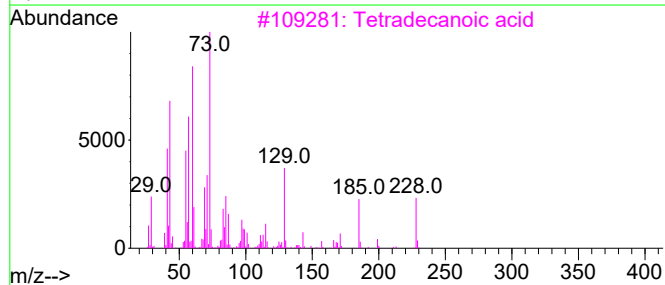
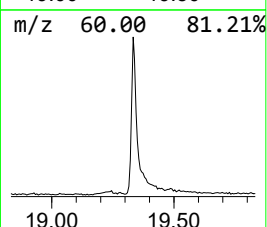
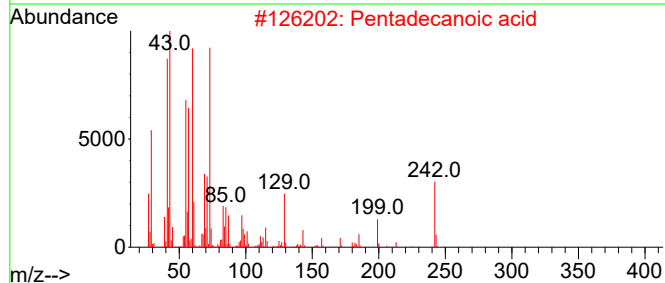
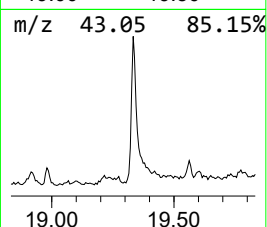
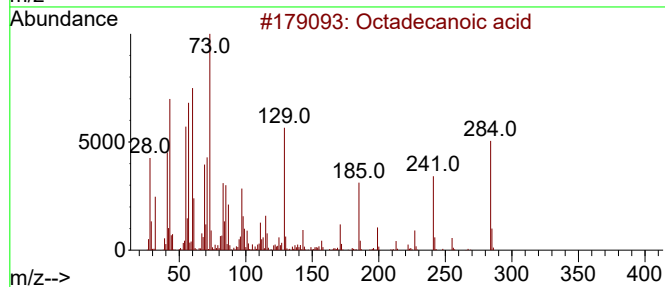
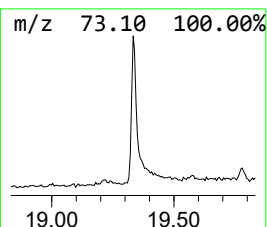
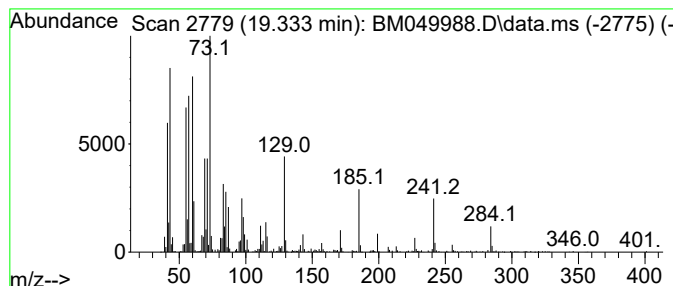
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.333	2.23 ng	808542	Chrysene-d12	21.397

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	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
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\BM042125\
Data File : BM049988.D
Acq On : 21 Apr 2025 17:11
Operator : RC/JU
Sample : Q1842-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PL-714-COMP-08

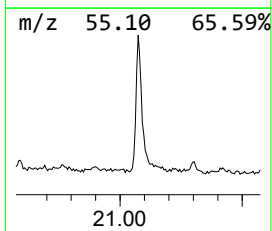
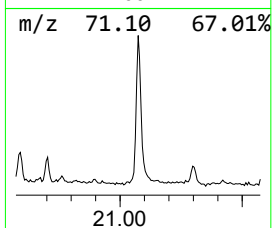
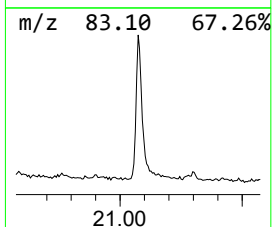
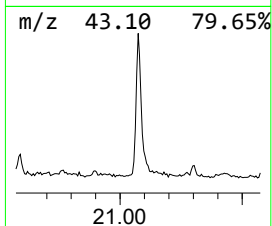
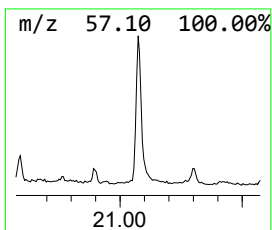
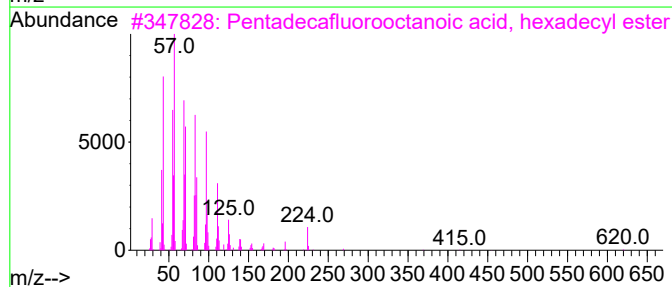
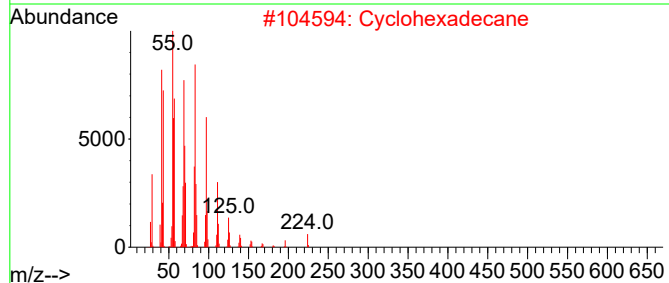
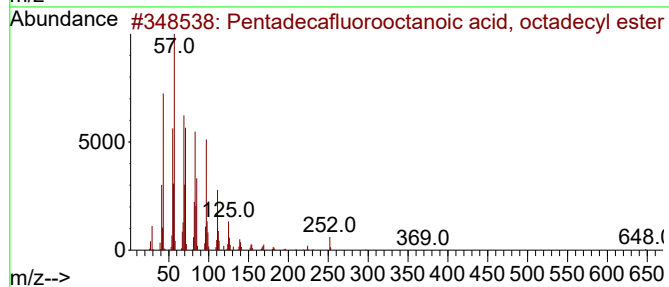
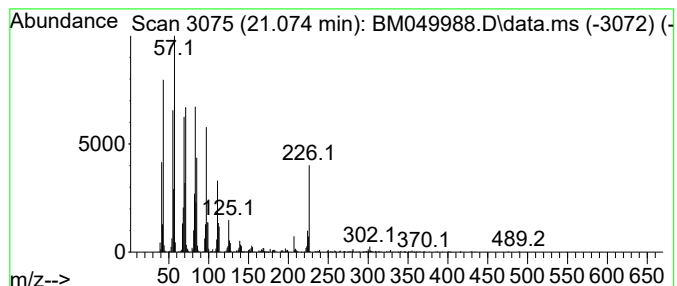
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.074	3.27 ng	1187790	Chrysene-d12	21.397

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
2			Cyclohexadecane	224	C16H32	000295-65-8	91
3			Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	89
4			Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	89
5			Cyclopentadecane	210	C15H30	000295-48-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042125\
Data File : BM049988.D
Acq On : 21 Apr 2025 17:11
Operator : RC/JU
Sample : Q1842-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PL-714-COMP-08

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.887	11.9	ng	1403060	1	7.763	2356800	20.0
2-Pentanone, 4-...	5.963	2.0	ng	239441	1	7.763	2356800	20.0
Benzophenone	15.768	11.3	ng	2510100	3	14.410	4452810	20.0
n-Hexadecanoic ...	18.056	11.7	ng	3233940	4	17.156	5537380	20.0
Octadecanoic acid	19.333	2.2	ng	808542	5	21.397	7256230	20.0
Pentadecafluoro...	21.074	3.3	ng	1187790	5	21.397	7256230	20.0