

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041025\
 Data File : BM049890.D
 Acq On : 10 Apr 2025 18:44
 Operator : RC/JU
 Sample : Q1748-05
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 IB-2A-WC

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: BM049890.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.893	319	324	336	rBV	905363	1240734	9.96%	1.478%
2	5.363	397	404	416	rBV	3923548	5708552	45.81%	6.799%
3	5.975	502	508	516	rVB	150037	223989	1.80%	0.267%
4	6.951	664	674	689	rBV	3866576	5984670	48.02%	7.127%
5	7.775	807	814	823	rBV	1174456	1795508	14.41%	2.138%
6	7.916	833	838	846	rVB	84970	134553	1.08%	0.160%
7	8.928	1003	1010	1020	rBV	2233984	3692751	29.63%	4.398%
8	10.569	1282	1289	1296	rBV	1431545	2394794	19.22%	2.852%
9	13.039	1701	1709	1718	rBV	6240887	8904707	71.45%	10.605%
10	14.416	1935	1943	1950	rBV	2390885	3487607	27.99%	4.154%
11	14.480	1950	1954	1962	rVB	108042	165796	1.33%	0.197%
12	15.463	2116	2121	2126	rBV	108212	157012	1.26%	0.187%
13	15.774	2167	2174	2181	rBV	1254297	1659417	13.32%	1.976%
14	15.904	2190	2196	2206	rBV	5858063	8345595	66.97%	9.939%
15	16.339	2266	2270	2276	rVB	137265	172089	1.38%	0.205%
16	17.162	2404	2410	2414	rBV2	2921885	4211826	33.80%	5.016%
17	17.204	2414	2417	2423	rVV	1170501	1560367	12.52%	1.858%
18	17.292	2423	2432	2438	rVB	270942	464201	3.72%	0.553%
19	17.562	2472	2478	2482	rBV2	110746	180248	1.45%	0.215%
20	18.062	2555	2563	2573	rBV2	588815	1301177	10.44%	1.550%
21	18.168	2577	2581	2586	rVV2	125349	230965	1.85%	0.275%
22	18.233	2587	2592	2596	rVV3	227434	438176	3.52%	0.522%
23	18.274	2596	2599	2605	rVB3	128657	249089	2.00%	0.297%
24	18.456	2625	2630	2634	rBV	577870	743481	5.97%	0.885%
25	18.645	2657	2662	2671	rVB2	238831	338872	2.72%	0.404%
26	19.215	2755	2759	2765	rBV	1521016	2030094	16.29%	2.418%
27	19.339	2777	2780	2788	rVB3	179967	253511	2.03%	0.302%
28	19.551	2812	2816	2817	rBV	282495	318408	2.55%	0.379%
29	19.580	2817	2821	2830	rVB	1263129	1819583	14.60%	2.167%
30	19.786	2851	2856	2861	rVB	10943759	12462311	100.00%	14.842%
31	19.998	2890	2892	2896	rVB	176618	193506	1.55%	0.230%
32	20.074	2902	2905	2909	rBV	235971	301420	2.42%	0.359%
33	20.180	2919	2923	2926	rBV	216693	286143	2.30%	0.341%
34	21.080	3072	3076	3094	rVB5	723738	1434259	11.51%	1.708%
35	21.397	3123	3130	3134	rBV2	3153982	5350253	42.93%	6.372%
36	21.439	3135	3137	3145	rVB	587160	727194	5.84%	0.866%

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041025\
Data File : BM049890.D
Acq On : 10 Apr 2025 18:44
Operator : RC/JU
Sample : Q1748-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
IB-2A-WC

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

37	24.391	3633	3639	3657	rVB	1881217	5004804	40.16%	5.960%
----	--------	------	------	------	-----	---------	---------	--------	--------

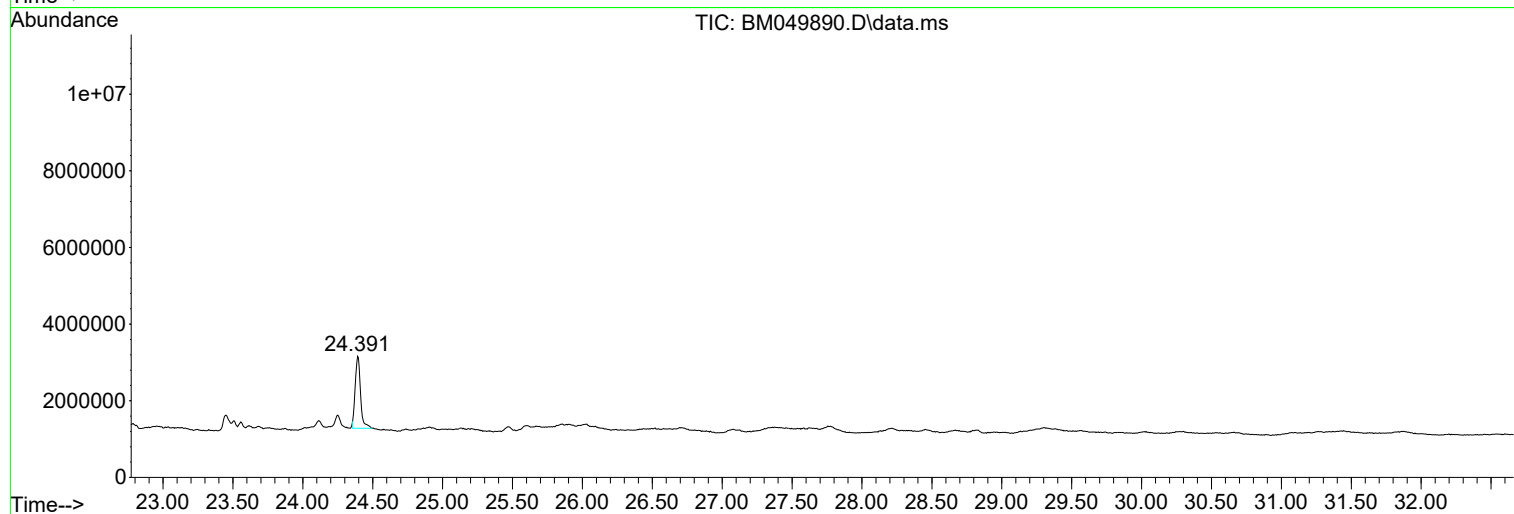
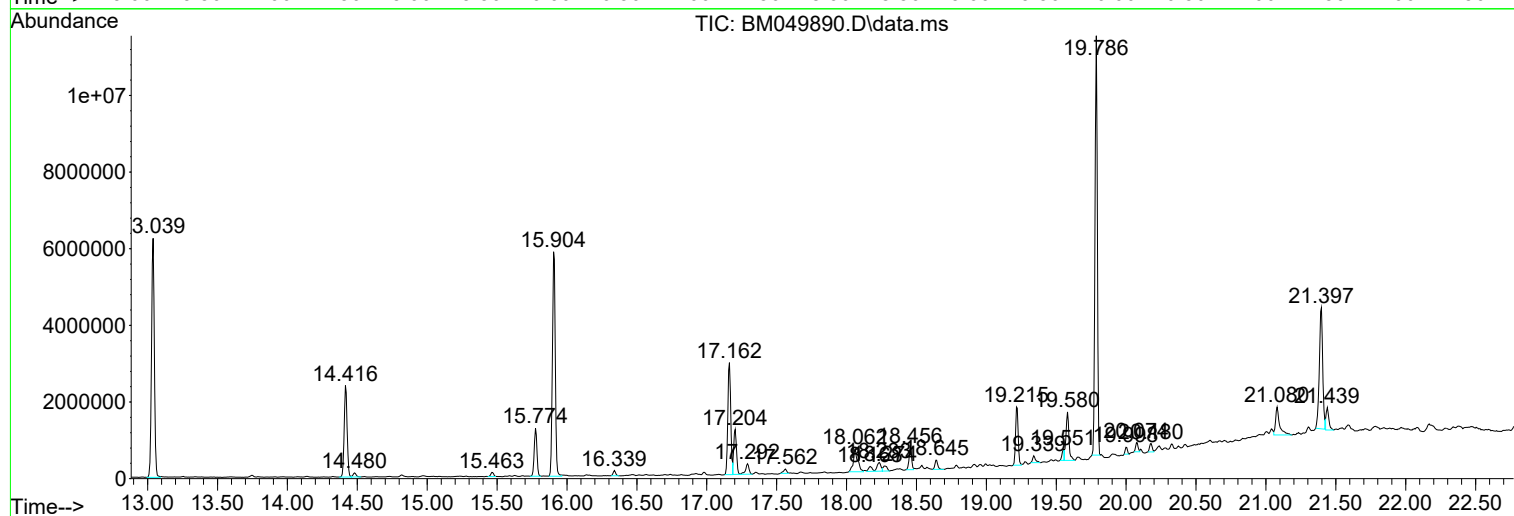
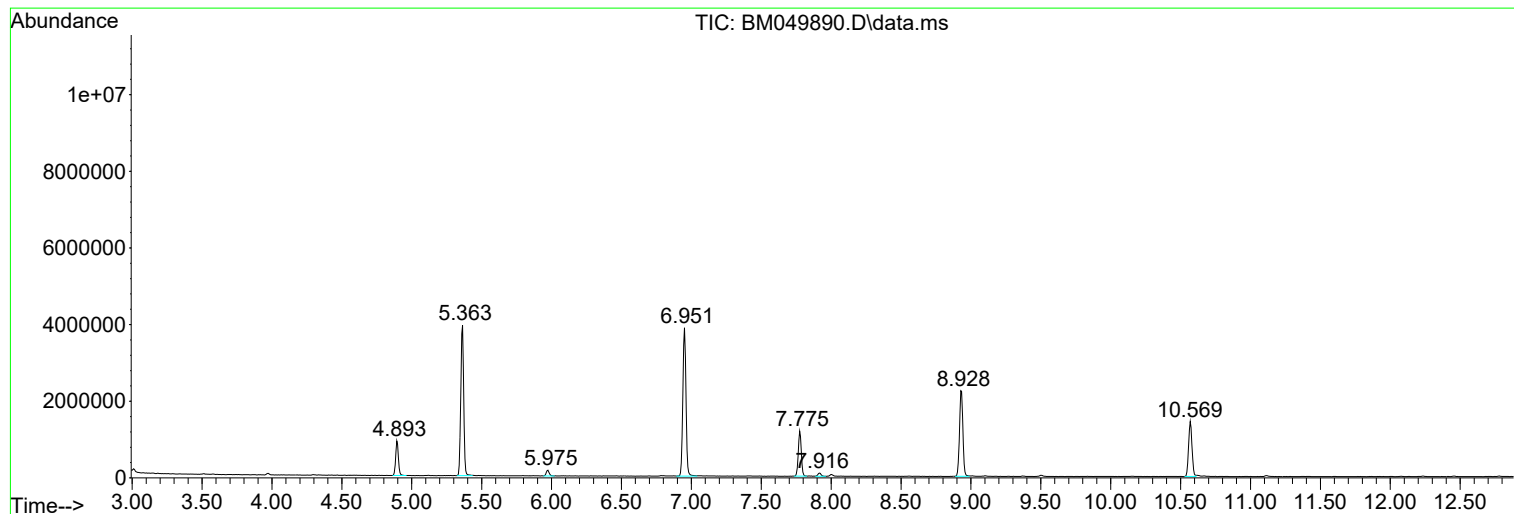
Sum of corrected areas: 83967662

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041025\
Data File : BM049890.D
Acq On : 10 Apr 2025 18:44
Operator : RC/JU
Sample : Q1748-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
IB-2A-WC

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\BM041025\
Data File : BM049890.D
Acq On : 10 Apr 2025 18:44
Operator : RC/JU
Sample : Q1748-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
IB-2A-WC

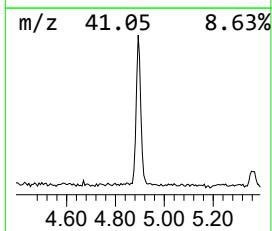
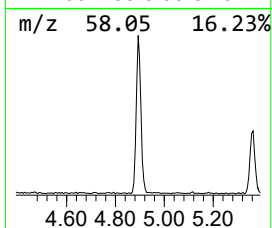
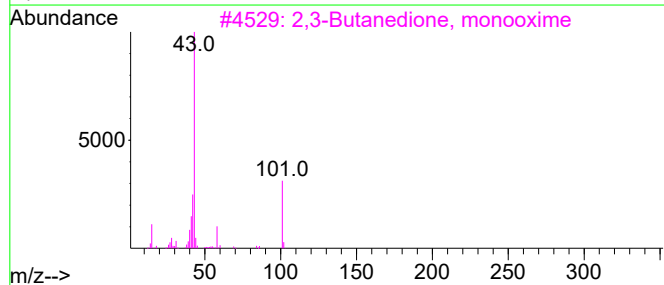
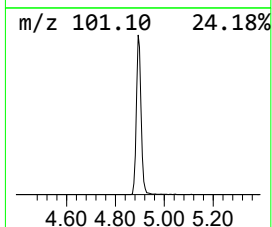
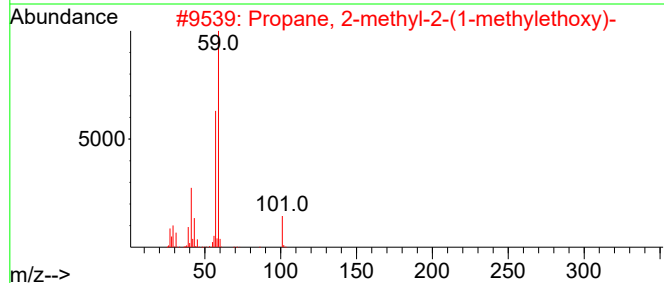
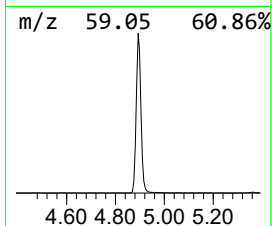
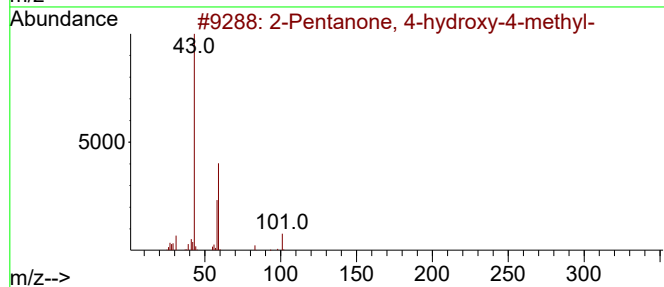
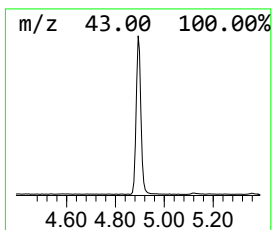
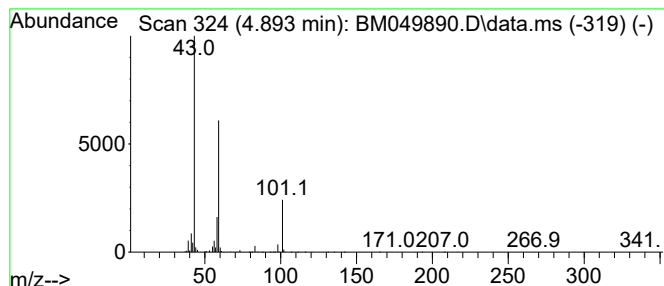
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.893	13.82 ng	1240730	1,4-Dichlorobenzene-d4	7.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041025\
Data File : BM049890.D
Acq On : 10 Apr 2025 18:44
Operator : RC/JU
Sample : Q1748-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
IB-2A-WC

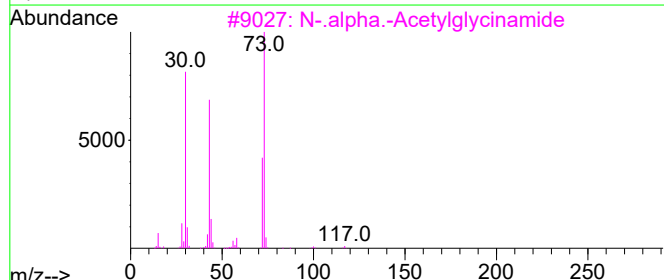
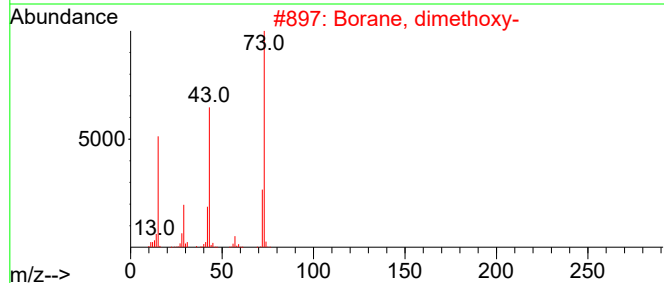
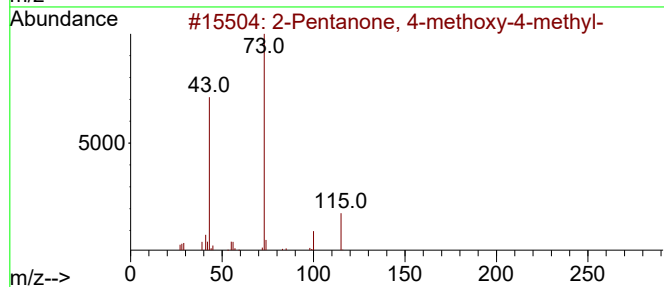
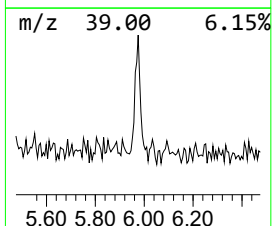
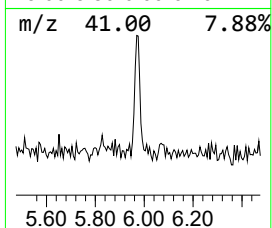
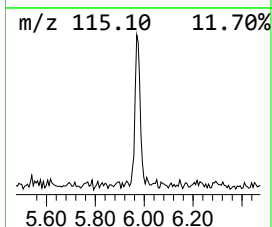
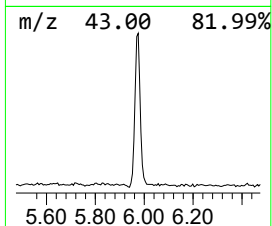
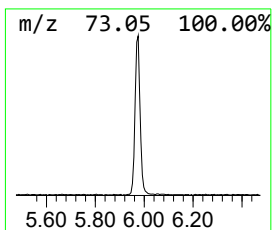
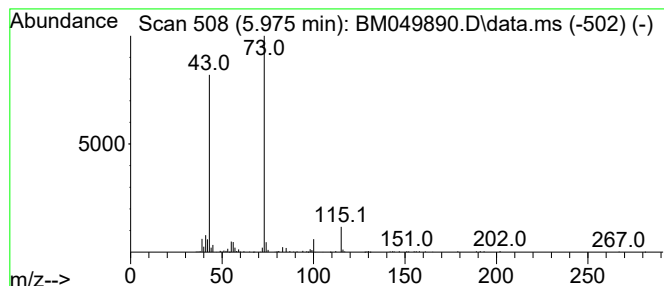
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.975	2.49 ng	223989	1,4-Dichlorobenzene-d4	7.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	38
3			N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	28
4			3-Heptanol, 3,5-dimethyl-	144	C9H20O	019549-74-7	25
5			4-Acetyoxytridecane	242	C15H30O2	060826-30-4	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041025\
Data File : BM049890.D
Acq On : 10 Apr 2025 18:44
Operator : RC/JU
Sample : Q1748-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
IB-2A-WC

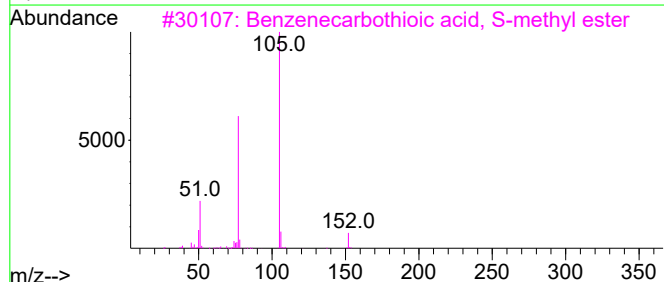
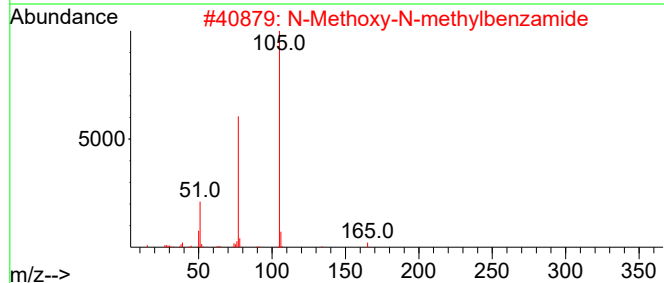
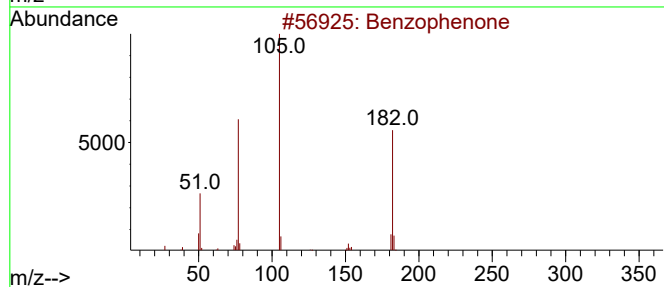
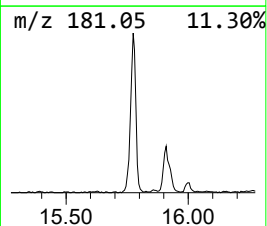
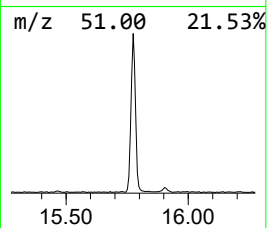
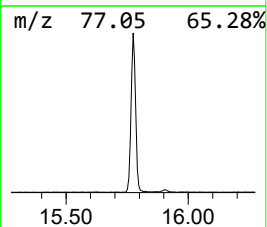
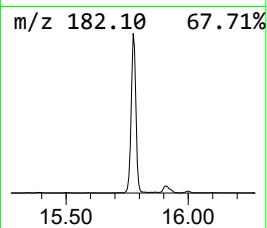
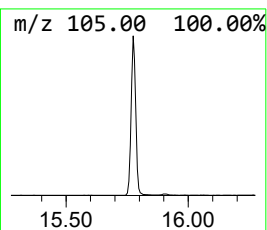
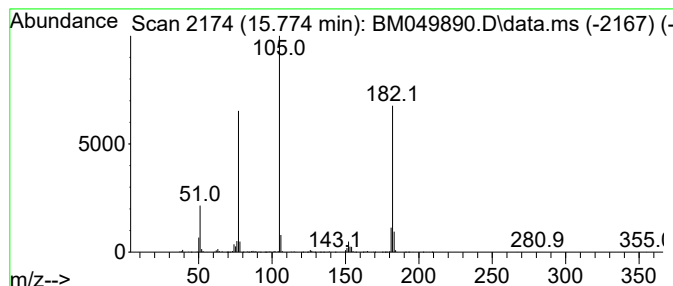
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
15.774	9.52 ng	1659420	Acenaphthene-d10	14.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	46
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	46
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041025\
Data File : BM049890.D
Acq On : 10 Apr 2025 18:44
Operator : RC/JU
Sample : Q1748-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
IB-2A-WC

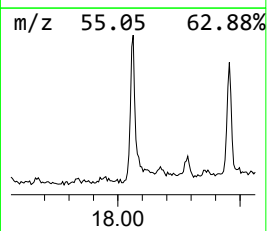
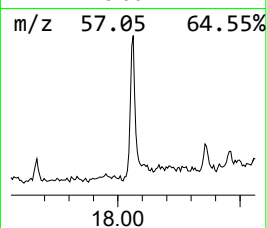
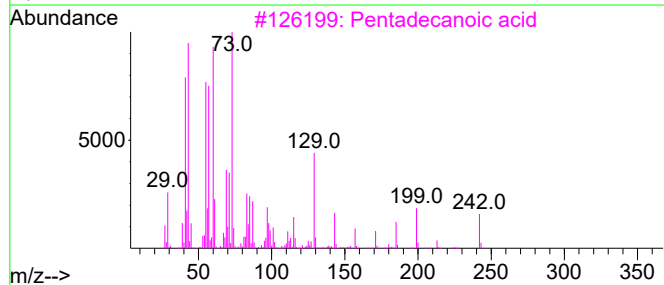
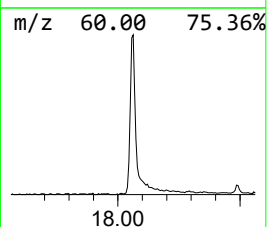
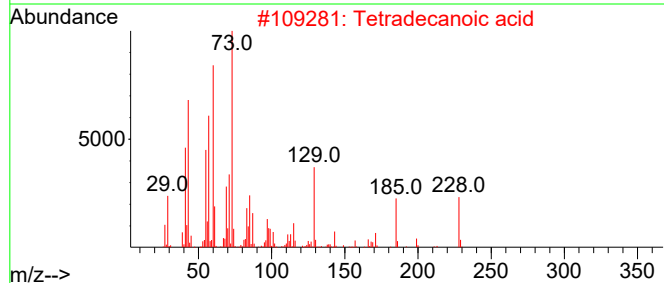
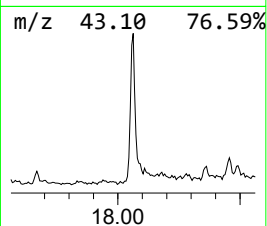
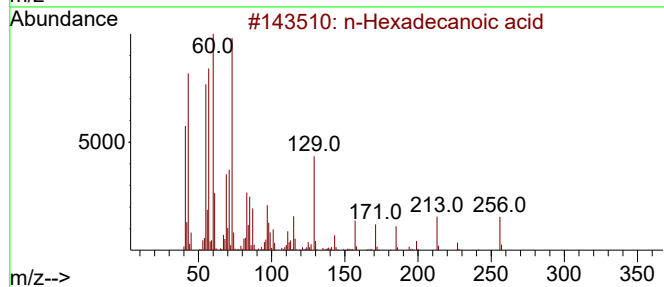
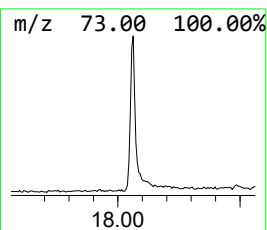
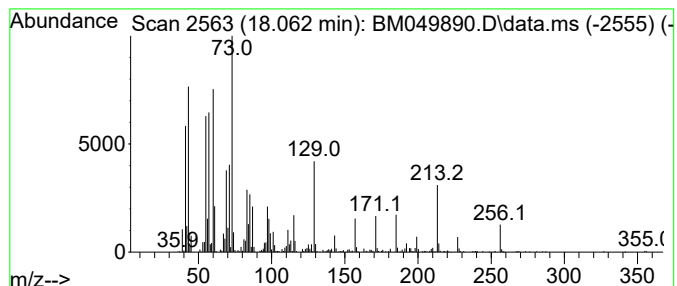
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.062	6.18 ng	1301180	Phenanthrene-d10	17.162

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	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Octadecanoic acid	284	C18H36O2	000057-11-4	90
5		Tridecanoic acid	214	C13H26O2	000638-53-9	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041025\
Data File : BM049890.D
Acq On : 10 Apr 2025 18:44
Operator : RC/JU
Sample : Q1748-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
IB-2A-WC

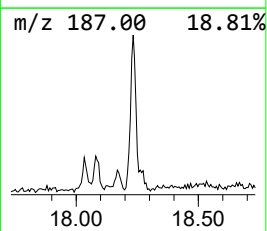
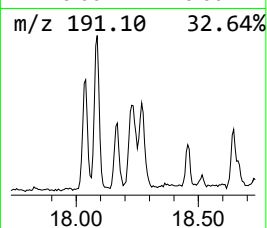
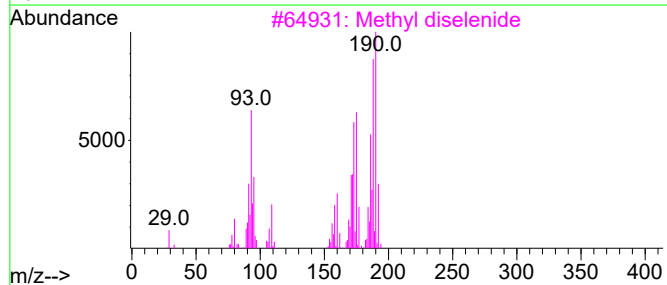
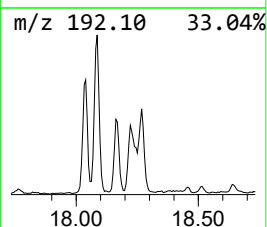
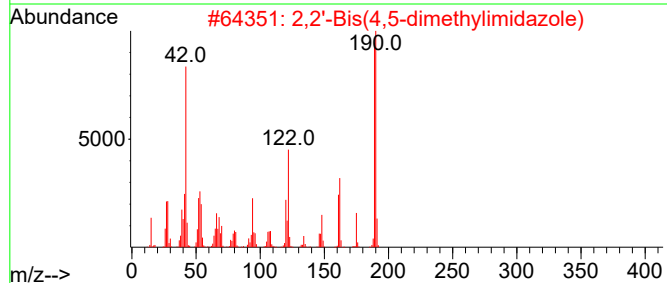
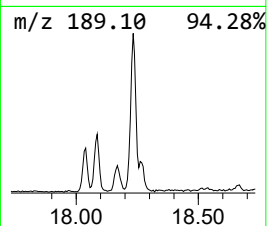
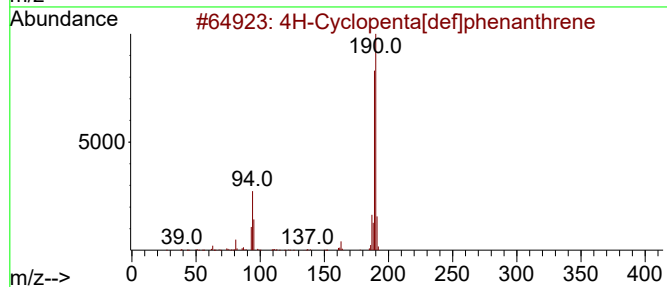
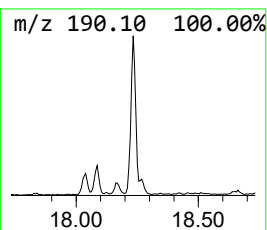
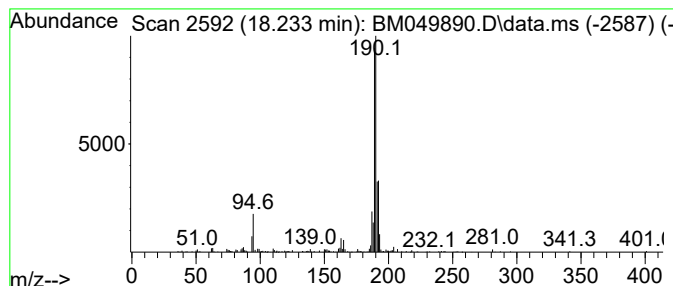
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	2.08 ng	438176	Phenanthrene-d10	17.162

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	83
2			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
3			Methyl diselenide	190	C2H6Se2	007101-31-7	35
4			Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	27
5			4-Isothiazolecarbonitrile, 5-chl...	190	C5H3ClN2S2	054798-93-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041025\
Data File : BM049890.D
Acq On : 10 Apr 2025 18:44
Operator : RC/JU
Sample : Q1748-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

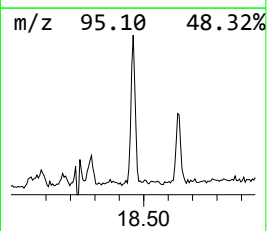
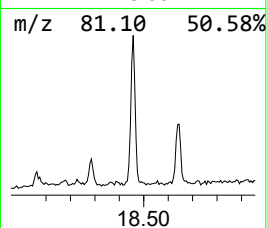
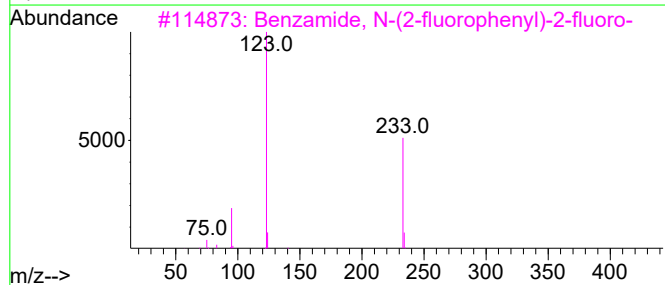
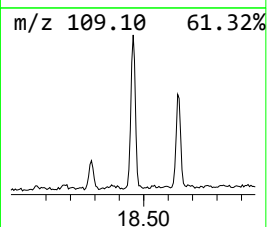
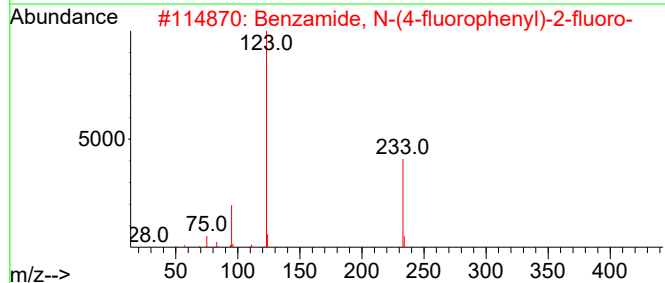
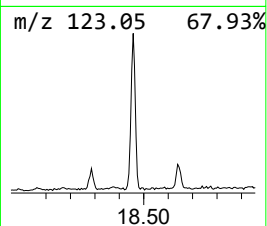
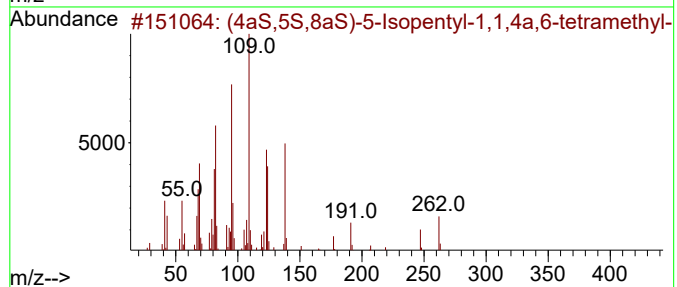
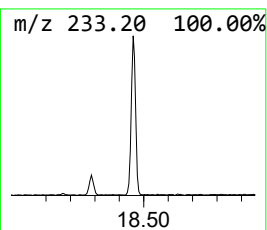
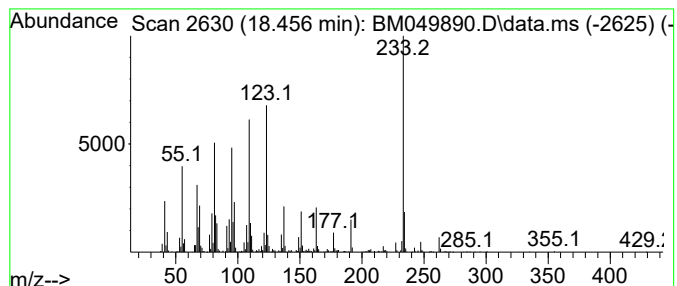
Instrument :
BNA_M
ClientSampleId :
IB-2A-WC

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 7 (4aS,5S,8aS)-5-Isopentyl-1,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.456	3.53 ng	743481	Phenanthrene-d10	17.162	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(4aS,5S,8aS)-5-Isopentyl-1,1,4a,...	262	C19H34	220766-81-4	58
2	Benzamide, N-(4-fluorophenyl)-2-...	233	C13H9F2NO	1000307-07-9	53
3	Benzamide, N-(2-fluorophenyl)-2-...	233	C13H9F2NO	1000308-09-1	49
4	Benzamide, N-(4-fluorophenyl)-4-...	233	C13H9F2NO	1000307-10-1	49
5	4H-1,2,4-triazole-3,5-diamine, N...	233	C11H12FN5	1000396-40-8	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041025\
Data File : BM049890.D
Acq On : 10 Apr 2025 18:44
Operator : RC/JU
Sample : Q1748-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
IB-2A-WC

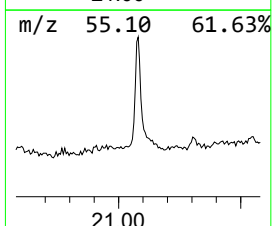
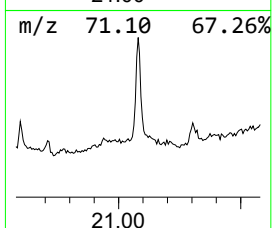
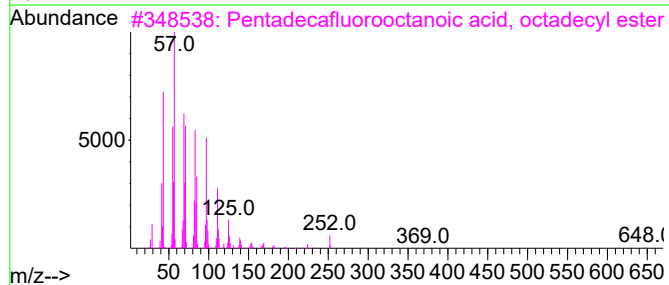
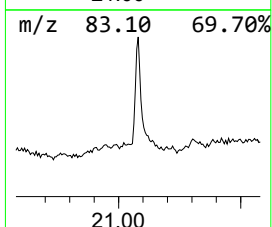
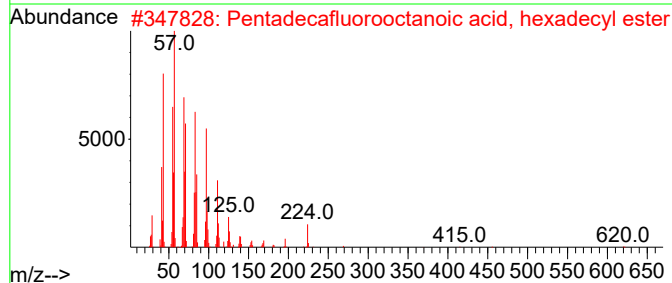
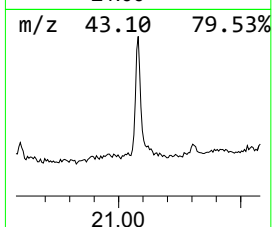
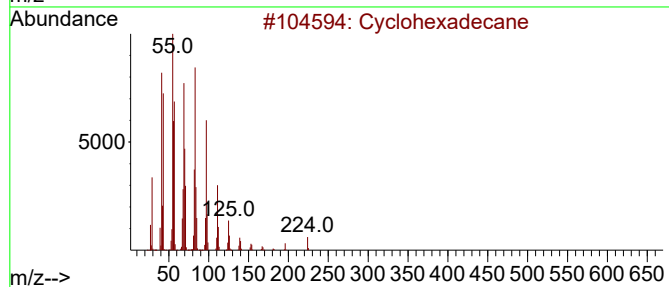
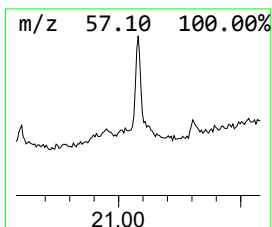
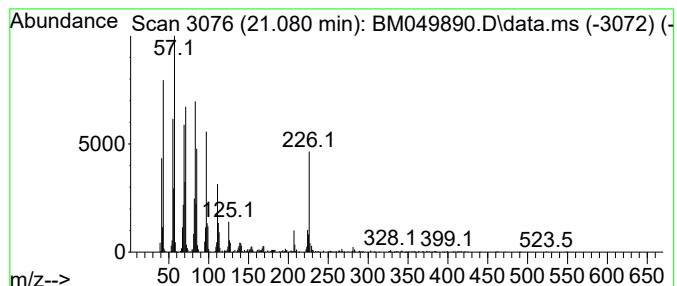
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.080	5.36 ng	1434260	Chrysene-d12	21.397

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	90
2			Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	89
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	86
4			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	81
5			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041025\
Data File : BM049890.D
Acq On : 10 Apr 2025 18:44
Operator : RC/JU
Sample : Q1748-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
IB-2A-WC

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
2-Pentanone, 4-...	4.893	13.8	ng	1240730	1	7.775	1795510	20.0
2-Pentanone, 4-...	5.975	2.5	ng	223989	1	7.775	1795510	20.0
Benzophenone	15.774	9.5	ng	1659420	3	14.416	3487610	20.0
n-Hexadecanoic ...	18.062	6.2	ng	1301180	4	17.162	4211830	20.0
4H-Cyclopenta[d...]	18.233	2.1	ng	438176	4	17.162	4211830	20.0
(4aS,5S,8aS)-5-...	18.456	3.5	ng	743481	4	17.162	4211830	20.0
Cyclohexadecane	21.080	5.4	ng	1434260	5	21.397	5350250	20.0