

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041825\
 Data File : BP024348.D
 Acq On : 18 Apr 2025 18:48
 Operator : RC/JU
 Sample : Q1828-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 RT4643

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_P\Methods\8270E-BP041425.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP024348.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	300	306	317	rBV	488794	674103	6.55%	1.002%
2	5.346	377	384	400	rBV	2497821	3739581	36.34%	5.559%
3	5.946	481	486	493	rBV	74023	107024	1.04%	0.159%
4	6.905	641	649	666	rBV	2385569	4066018	39.51%	6.044%
5	7.722	779	788	796	rBV	877489	1373152	13.34%	2.041%
6	8.869	975	983	1001	rBV	1615263	2592786	25.19%	3.854%
7	10.493	1251	1259	1272	rBV	1253961	1940870	18.86%	2.885%
8	12.963	1670	1679	1691	rBV	4199719	6195904	60.21%	9.211%
9	14.351	1907	1915	1921	rBV	1819781	2502714	24.32%	3.720%
10	15.187	2050	2057	2062	rBV	154227	275271	2.67%	0.409%
11	15.734	2142	2150	2163	rBV	1103061	1592628	15.48%	2.368%
12	15.869	2166	2173	2182	rBV	3636743	5178290	50.32%	7.698%
13	16.310	2243	2248	2255	rVB	117098	165906	1.61%	0.247%
14	17.145	2384	2390	2395	rBV2	2077247	3015114	29.30%	4.482%
15	17.186	2395	2397	2405	rVB	247302	330911	3.22%	0.492%
16	18.092	2546	2551	2559	rBV2	972326	1451792	14.11%	2.158%
17	19.275	2747	2752	2762	rBV	947297	1343902	13.06%	1.998%
18	19.416	2772	2776	2792	rBV2	550084	929418	9.03%	1.382%
19	19.651	2807	2816	2821	rBV	794804	1263227	12.28%	1.878%
20	19.875	2848	2854	2866	rVB	7543866	10290994	100.00%	15.298%
21	20.333	2929	2932	2937	rVB3	82239	111912	1.09%	0.166%
22	20.686	2989	2992	2995	rVB	112334	117919	1.15%	0.175%
23	21.263	3087	3090	3107	rVB4	282103	771214	7.49%	1.146%
24	21.580	3137	3144	3150	rBV3	2354053	4523926	43.96%	6.725%
25	21.633	3150	3153	3165	rVB	434371	678230	6.59%	1.008%
26	22.874	3357	3364	3374	rBV	4131563	6913045	67.18%	10.277%
27	23.874	3528	3534	3542	rBV	275365	814407	7.91%	1.211%
28	24.068	3565	3567	3575	rVB3	167908	297634	2.89%	0.442%
29	24.933	3705	3714	3725	rBV	1445520	4010671	38.97%	5.962%

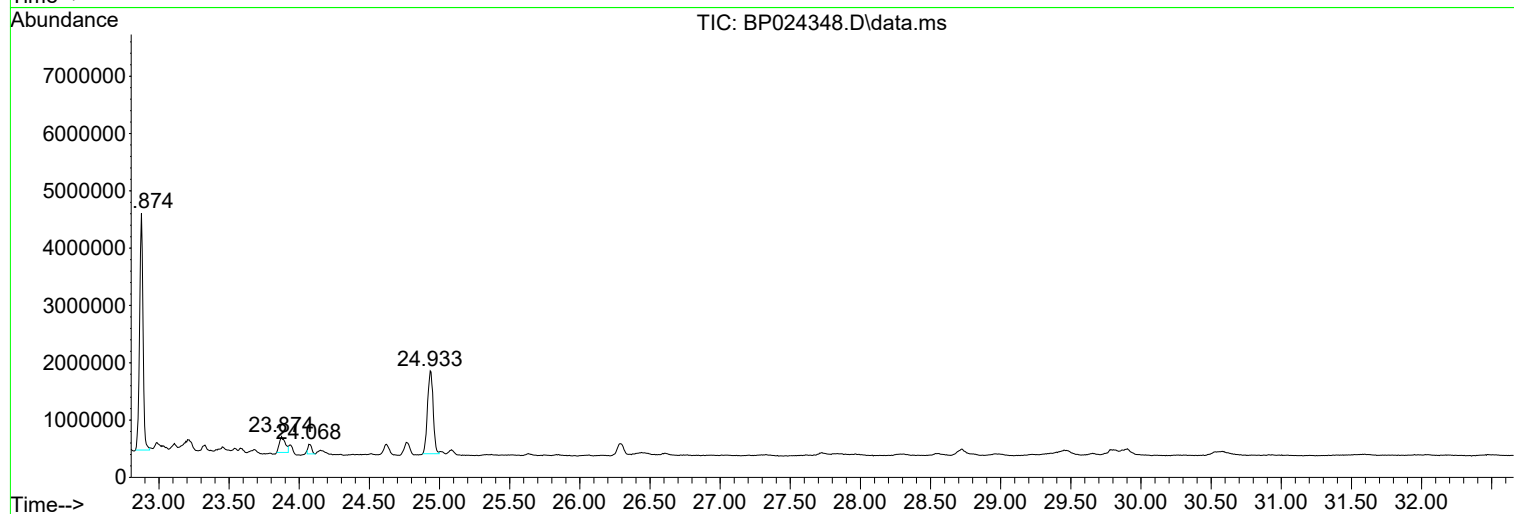
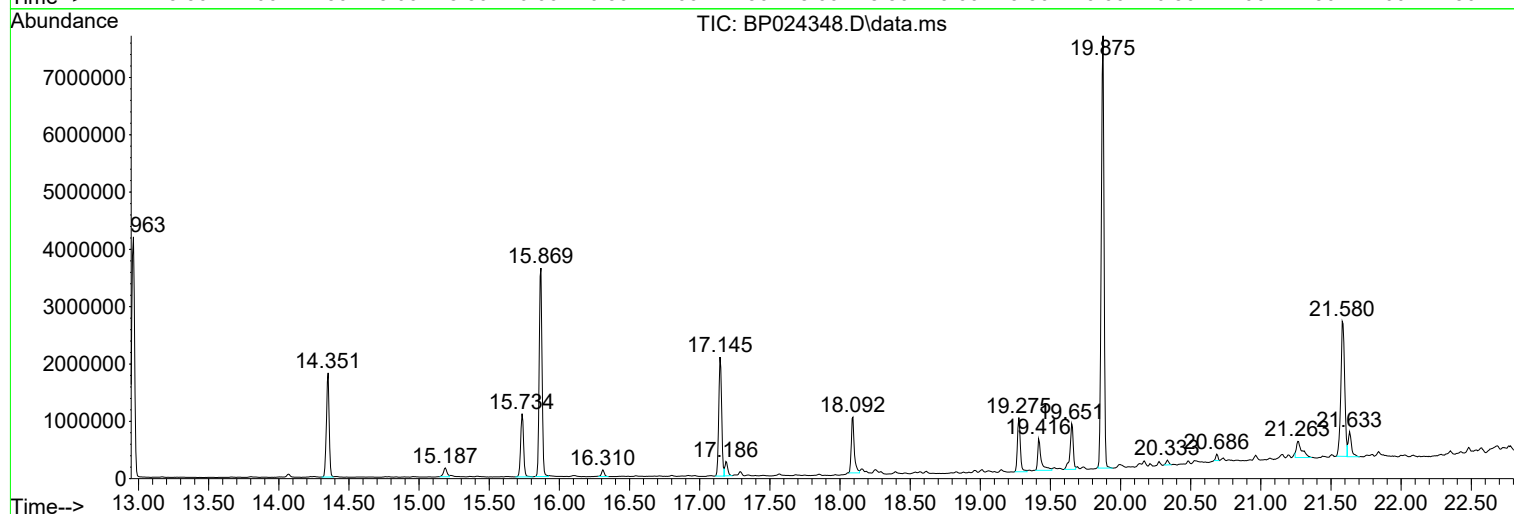
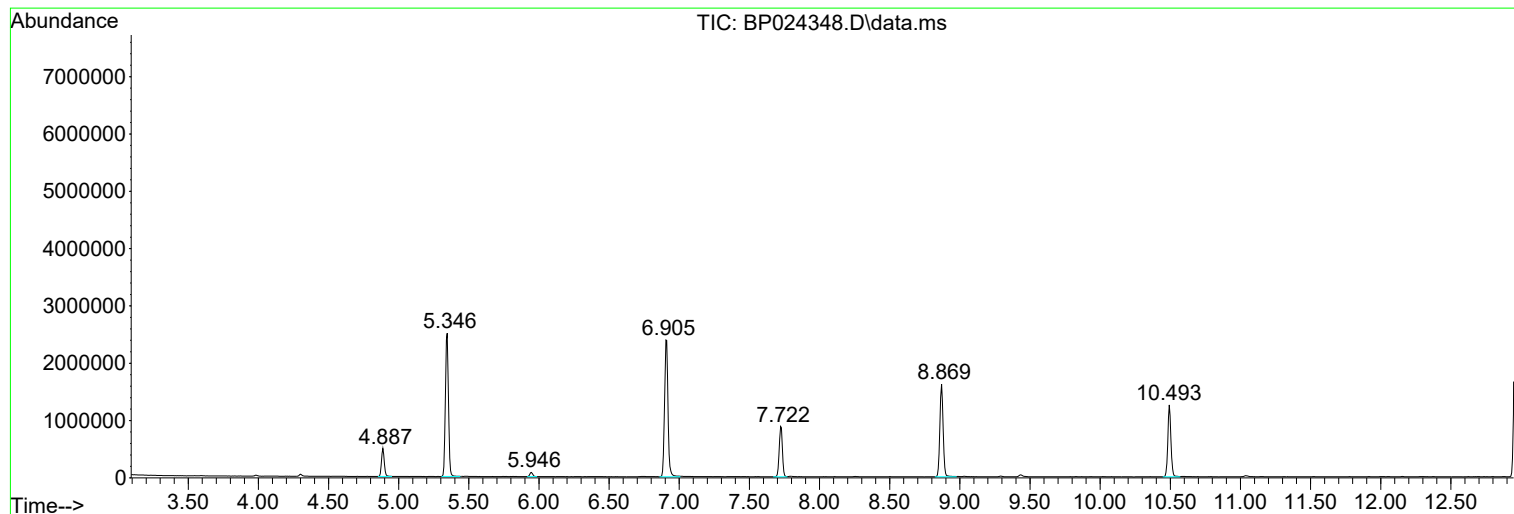
Sum of corrected areas: 67268563

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041825\
Data File : BP024348.D
Acq On : 18 Apr 2025 18:48
Operator : RC/JU
Sample : Q1828-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RT4643

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.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_P\Data\BP041825\
Data File : BP024348.D
Acq On : 18 Apr 2025 18:48
Operator : RC/JU
Sample : Q1828-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RT4643

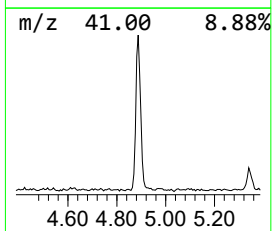
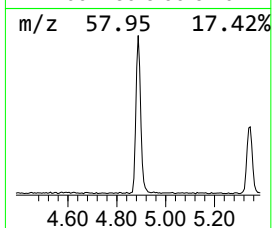
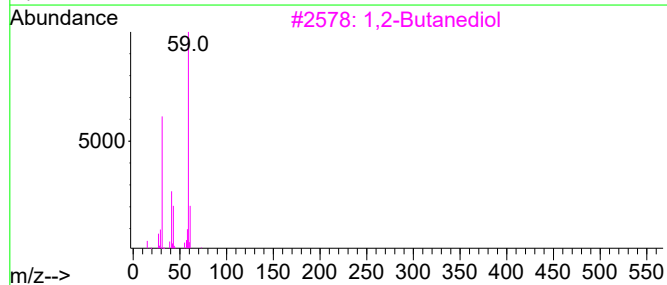
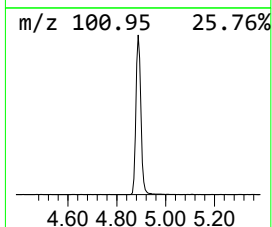
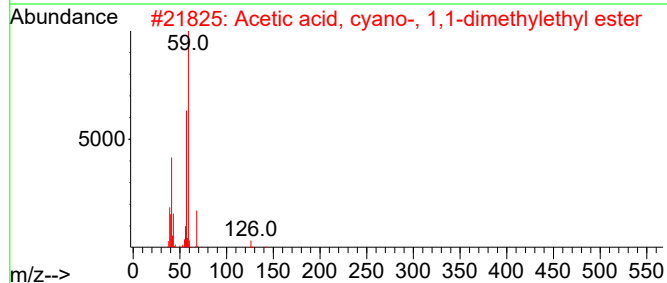
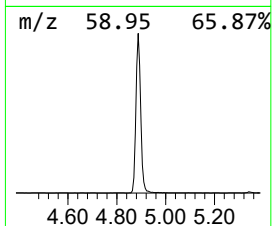
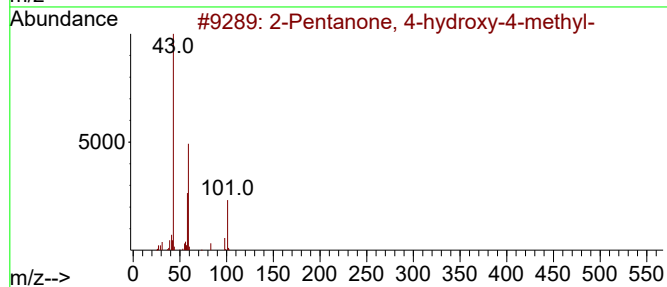
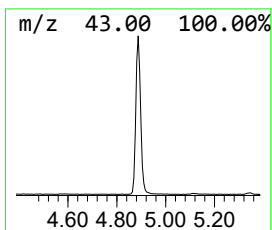
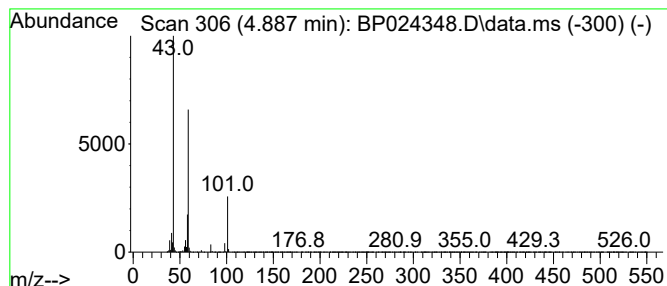
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.887	9.82 ng	674103	1,4-Dichlorobenzene-d4	7.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
3	1,2-Butanediol	90	C4H10O2	000584-03-2	17		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041825\
Data File : BP024348.D
Acq On : 18 Apr 2025 18:48
Operator : RC/JU
Sample : Q1828-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RT4643

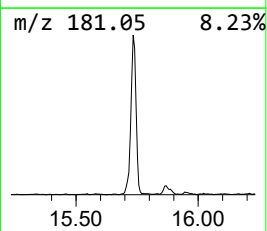
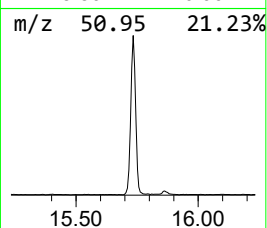
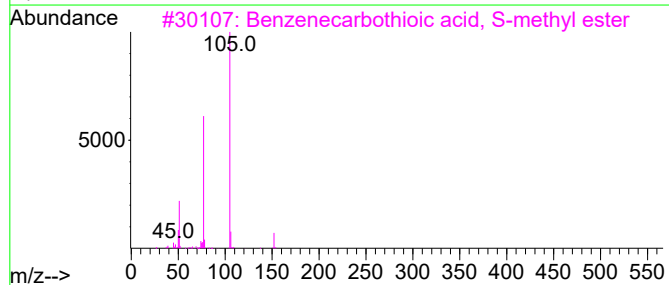
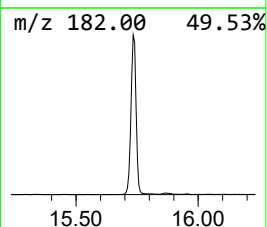
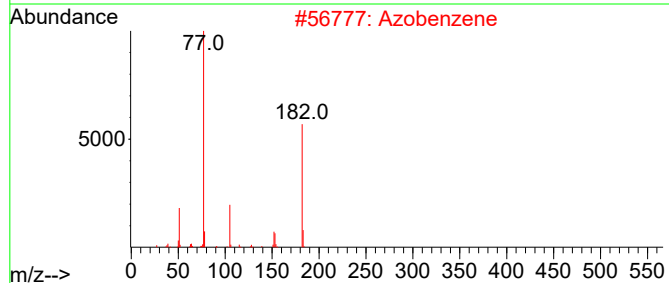
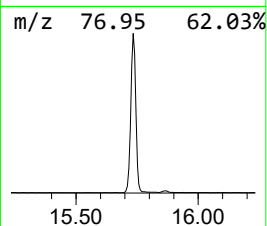
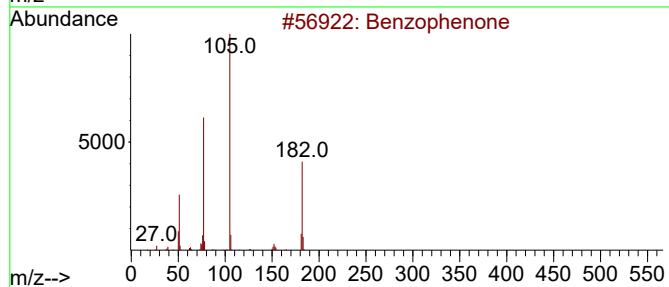
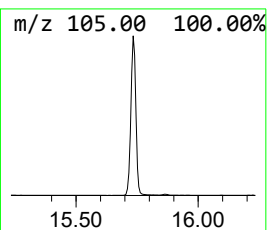
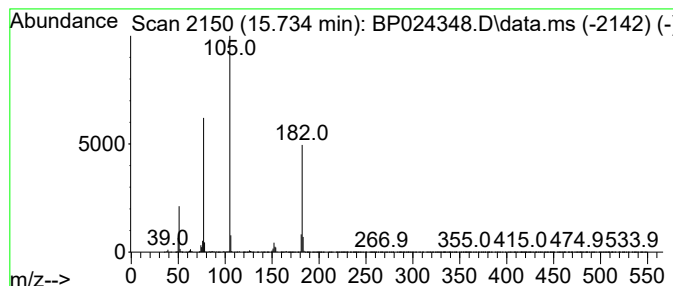
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.734	12.73 ng	1592630	Acenaphthene-d10	14.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Azobenzene	182	C12H10N2	000103-33-3	64
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
4			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
5			Vinyl benzoate	148	C9H8O2	000769-78-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041825\
Data File : BP024348.D
Acq On : 18 Apr 2025 18:48
Operator : RC/JU
Sample : Q1828-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RT4643

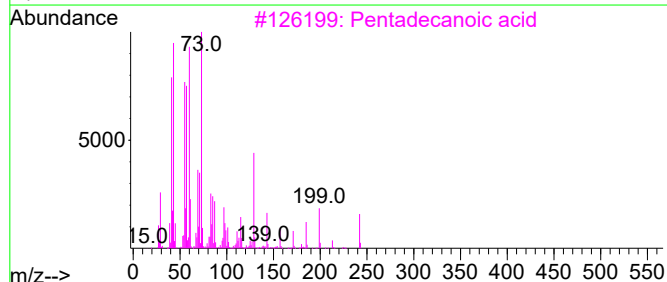
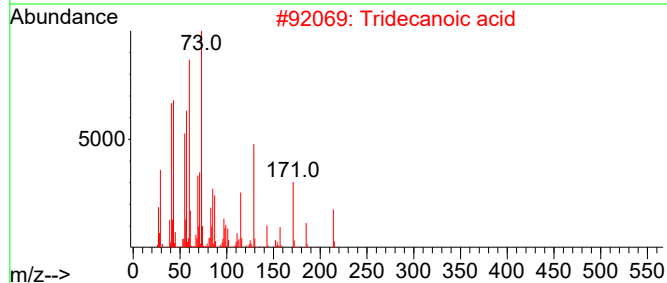
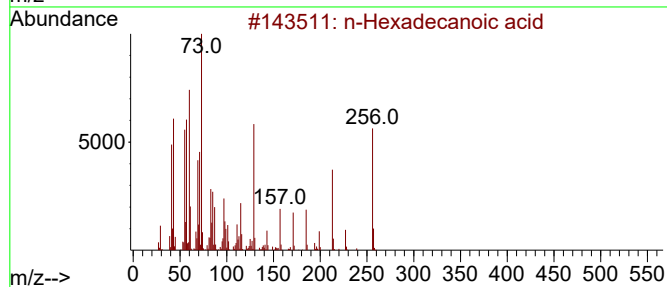
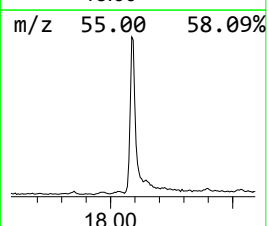
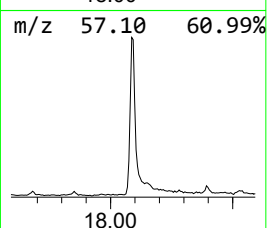
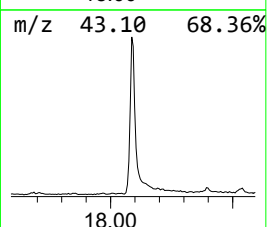
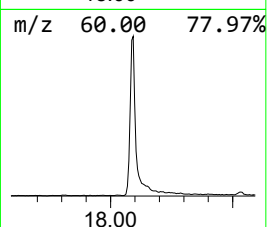
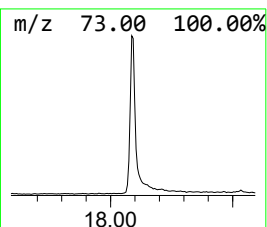
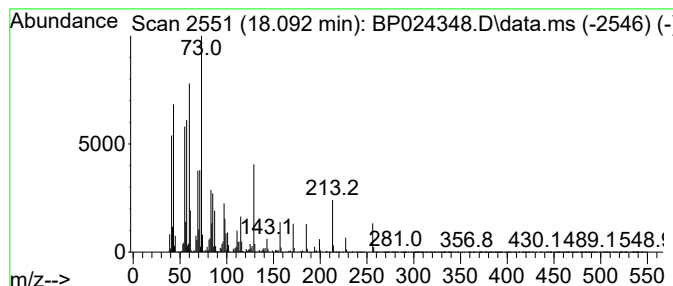
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.092	9.63 ng	1451790	Phenanthrene-d10	17.145

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041825\
Data File : BP024348.D
Acq On : 18 Apr 2025 18:48
Operator : RC/JU
Sample : Q1828-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RT4643

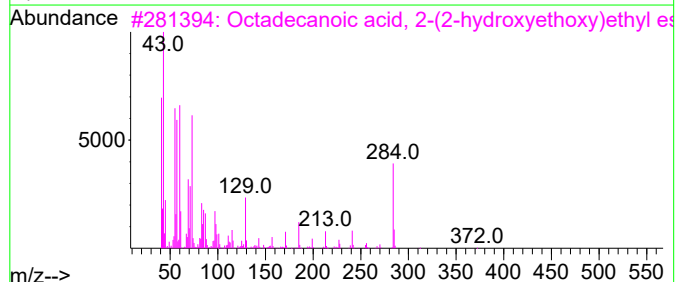
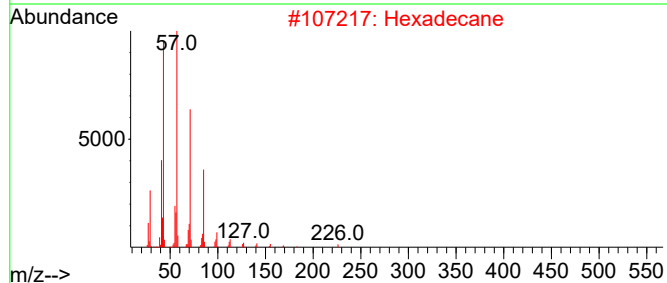
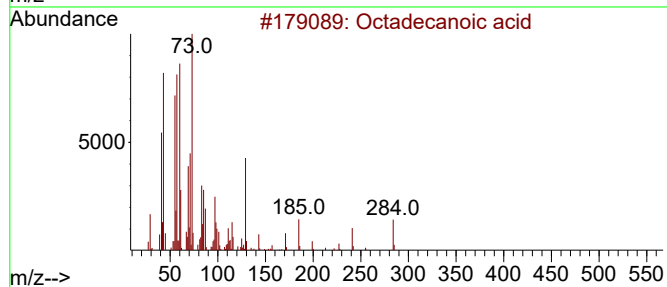
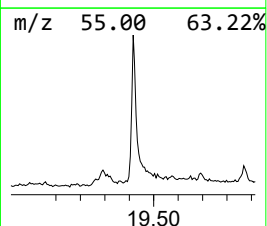
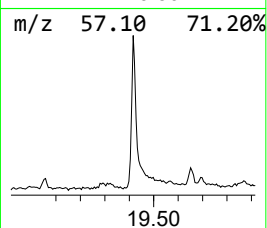
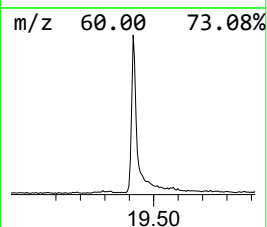
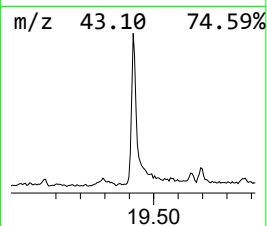
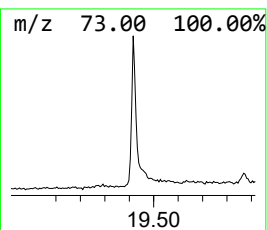
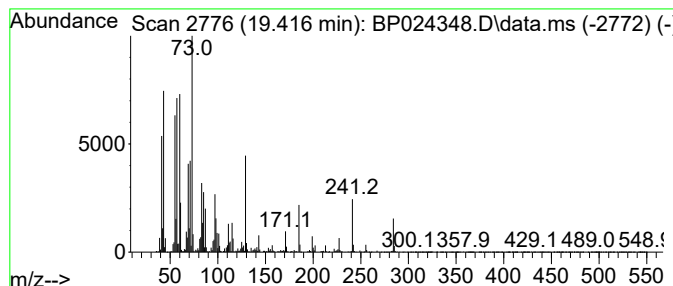
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.416	4.11 ng	929418	Chrysene-d12	21.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Hexadecane	226	C16H34	000544-76-3	90
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041825\
Data File : BP024348.D
Acq On : 18 Apr 2025 18:48
Operator : RC/JU
Sample : Q1828-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RT4643

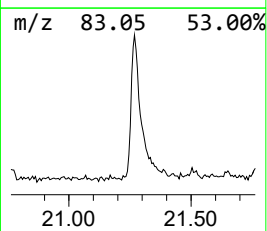
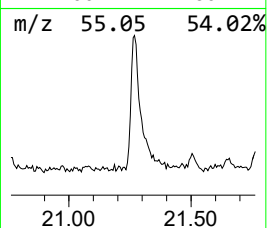
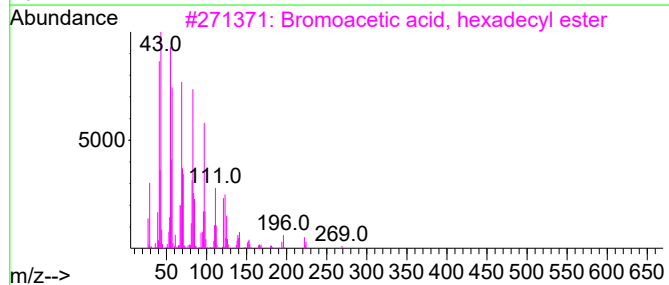
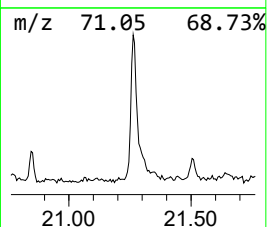
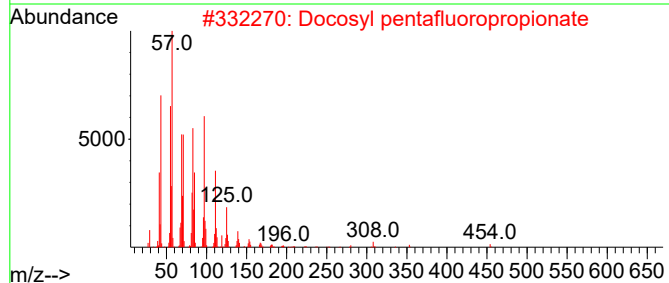
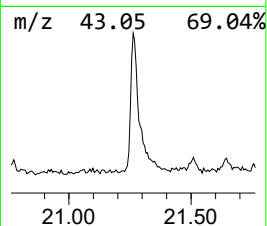
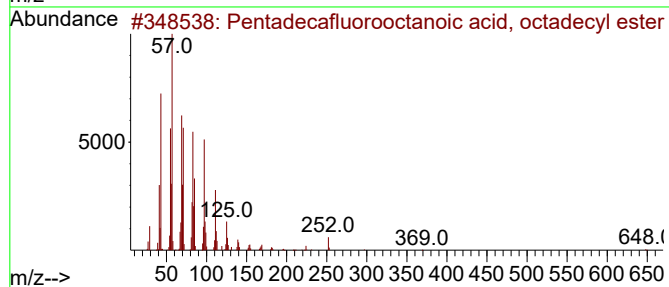
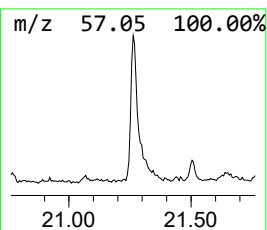
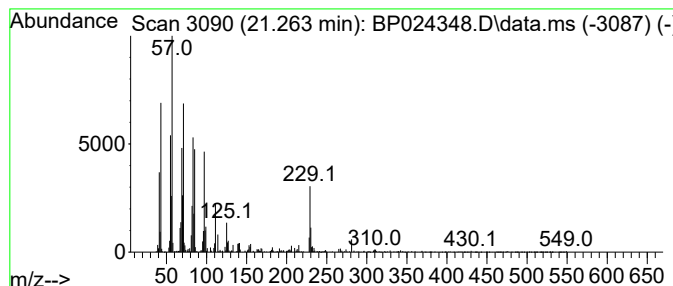
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.263	3.41 ng	771214	Chrysene-d12	21.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	92
2			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	62
3			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	60
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	60
5			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041825\
Data File : BP024348.D
Acq On : 18 Apr 2025 18:48
Operator : RC/JU
Sample : Q1828-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RT4643

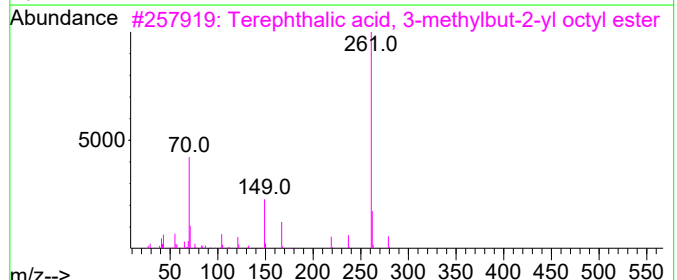
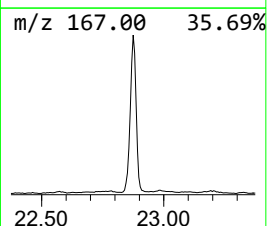
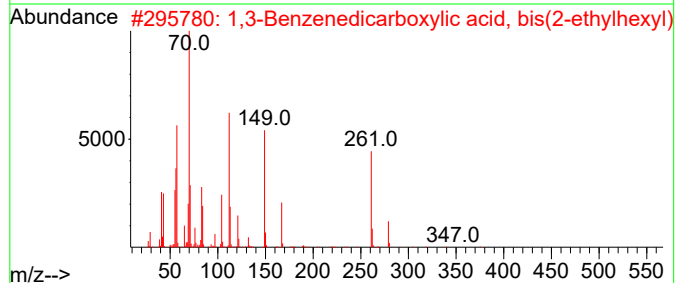
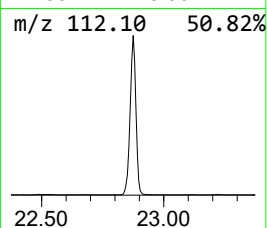
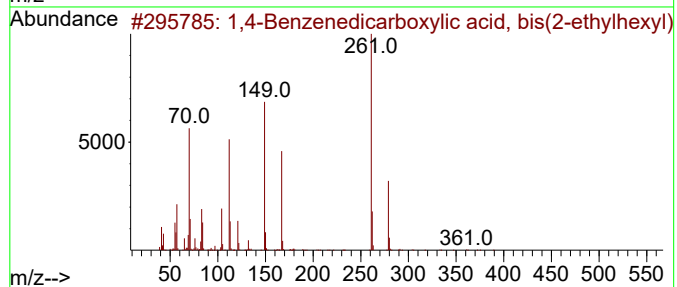
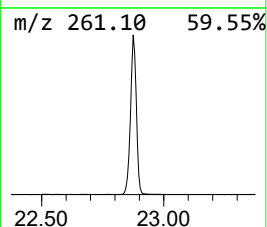
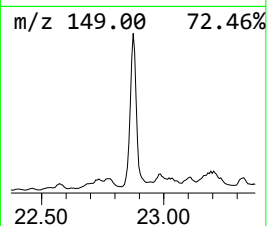
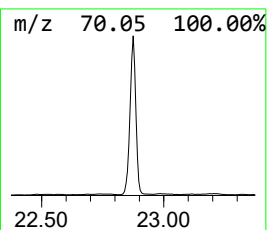
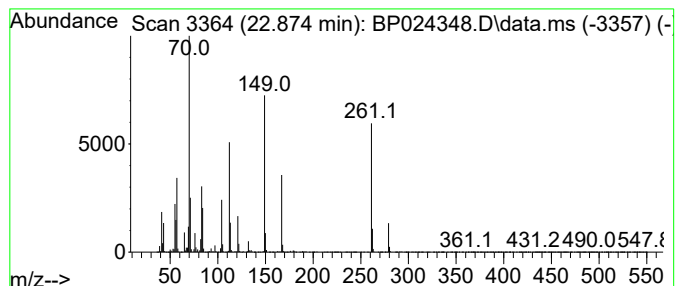
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.874	30.56 ng	6913050	Chrysene-d12	21.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	91
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	72
3			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	49
4			Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	43
5			Terephthalic acid, 3-hexyl octyl...	362	C22H34O4	1000356-23-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041825\
Data File : BP024348.D
Acq On : 18 Apr 2025 18:48
Operator : RC/JU
Sample : Q1828-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RT4643

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.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	9.8	ng	674103	1	7.722	1373150	20.0
Benzophenone	15.734	12.7	ng	1592630	3	14.351	2502710	20.0
n-Hexadecanoic ...	18.092	9.6	ng	1451790	4	17.145	3015110	20.0
Octadecanoic acid	19.416	4.1	ng	929418	5	21.580	4523930	20.0
Pentadecafluoro...	21.263	3.4	ng	771214	5	21.580	4523930	20.0
1,4-Benzenedica...	22.874	30.6	ng	6913050	5	21.580	4523930	20.0