

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050125\
 Data File : BF142268.D
 Acq On : 01 May 2025 18:55
 Operator : RC/JU
 Sample : Q1901-02
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-167-SB01

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_F\Methods\8270-BF043025.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142268.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.316	14	21	31	rVB2	61821	104032	2.03%	0.288%
2	5.128	490	499	509	rVB	345774	542647	10.60%	1.501%
3	5.522	559	566	571	rBV	3123242	4406681	86.11%	12.190%
4	6.522	729	736	741	rBV	3210981	4586593	89.63%	12.687%
5	6.904	796	801	806	rVB	990793	1212302	23.69%	3.353%
6	7.463	890	896	901	rBV	2146315	2809135	54.90%	7.771%
7	7.716	935	939	943	rVB	51601	60763	1.19%	0.168%
8	8.187	1013	1019	1027	rBV	1279895	1580689	30.89%	4.372%
9	9.263	1196	1202	1207	rBV	4041357	5117237	100.00%	14.155%
10	9.939	1312	1317	1322	rBV	1272498	1557655	30.44%	4.309%
11	10.651	1433	1438	1443	rBV	590376	733968	14.34%	2.030%
12	10.728	1445	1451	1456	rBV	1932792	2429783	47.48%	6.721%
13	10.963	1482	1491	1495	rBV	37701	52475	1.03%	0.145%
14	11.428	1565	1570	1578	rBV2	1024684	1466179	28.65%	4.056%
15	11.498	1578	1582	1586	rVB	41975	54469	1.06%	0.151%
16	11.651	1603	1608	1617	rBV	171831	241763	4.72%	0.669%
17	11.951	1651	1659	1664	rBV2	186717	300023	5.86%	0.830%
18	12.039	1670	1674	1684	rVB	41160	78544	1.53%	0.217%
19	12.210	1698	1703	1714	rVB2	293250	401290	7.84%	1.110%
20	12.639	1771	1776	1782	rBV	218200	277995	5.43%	0.769%
21	12.733	1788	1792	1799	rBV2	54708	83843	1.64%	0.232%
22	12.869	1808	1815	1821	rBV	229100	324972	6.35%	0.899%
23	13.016	1834	1840	1845	rVB	2998466	3849663	75.23%	10.649%
24	13.910	1988	1992	2002	rVB	152371	230126	4.50%	0.637%
25	14.063	2012	2018	2031	rVB2	991615	1542539	30.14%	4.267%
26	14.545	2095	2100	2103	rBV3	43592	65918	1.29%	0.182%
27	14.939	2162	2167	2176	rVV2	42308	71962	1.41%	0.199%
28	15.116	2192	2197	2208	rBV	105644	249724	4.88%	0.691%
29	15.221	2209	2215	2222	rVB3	26927	66167	1.29%	0.183%
30	15.427	2245	2250	2255	rBV	60169	90811	1.77%	0.251%
31	15.486	2256	2260	2266	rVV	77408	114728	2.24%	0.317%
32	15.557	2266	2272	2289	rVB	798337	1282112	25.05%	3.547%
33	16.098	2361	2364	2374	rVB4	27687	56638	1.11%	0.157%
34	17.051	2522	2526	2535	rVB2	24909	51275	1.00%	0.142%
35	17.498	2598	2602	2613	rVB2	24012	56045	1.10%	0.155%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050125\
Data File : BF142268.D
Acq On : 01 May 2025 18:55
Operator : RC/JU
Sample : Q1901-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-167-SB01

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_F\Methods\8270-BF043025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

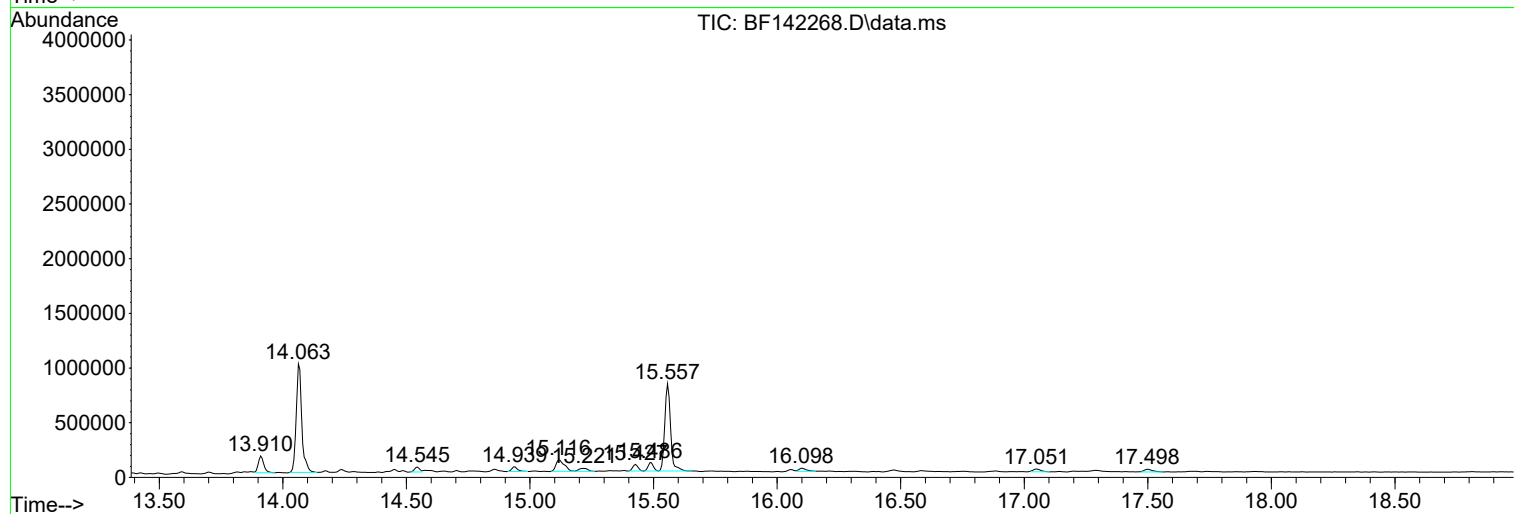
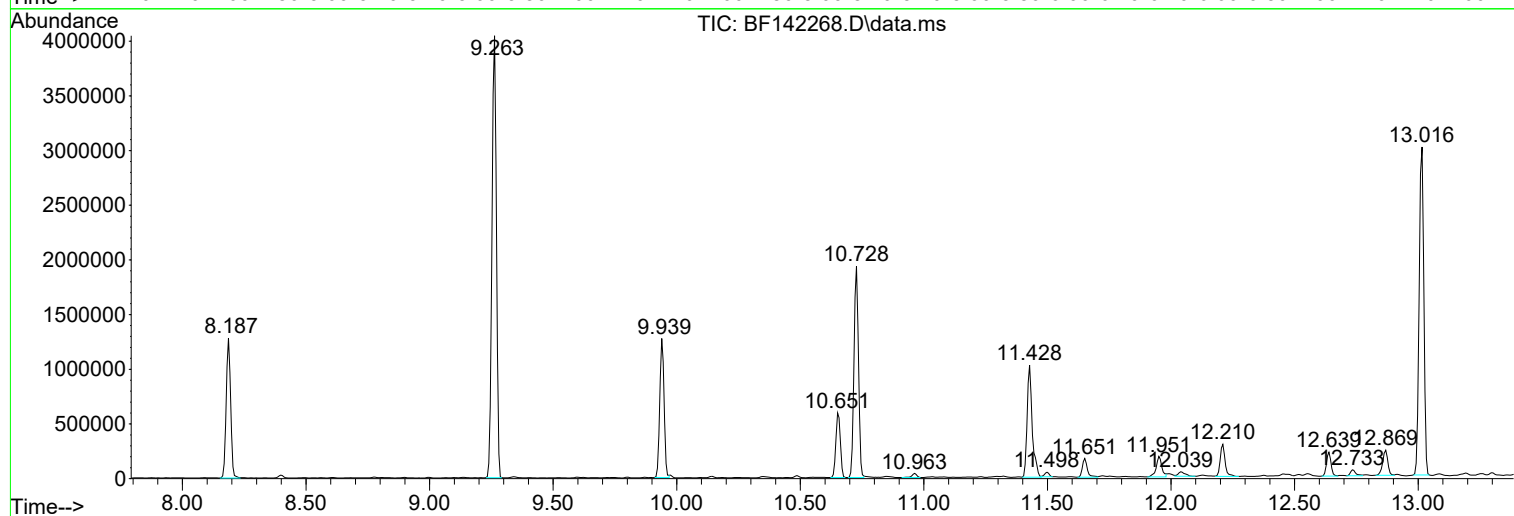
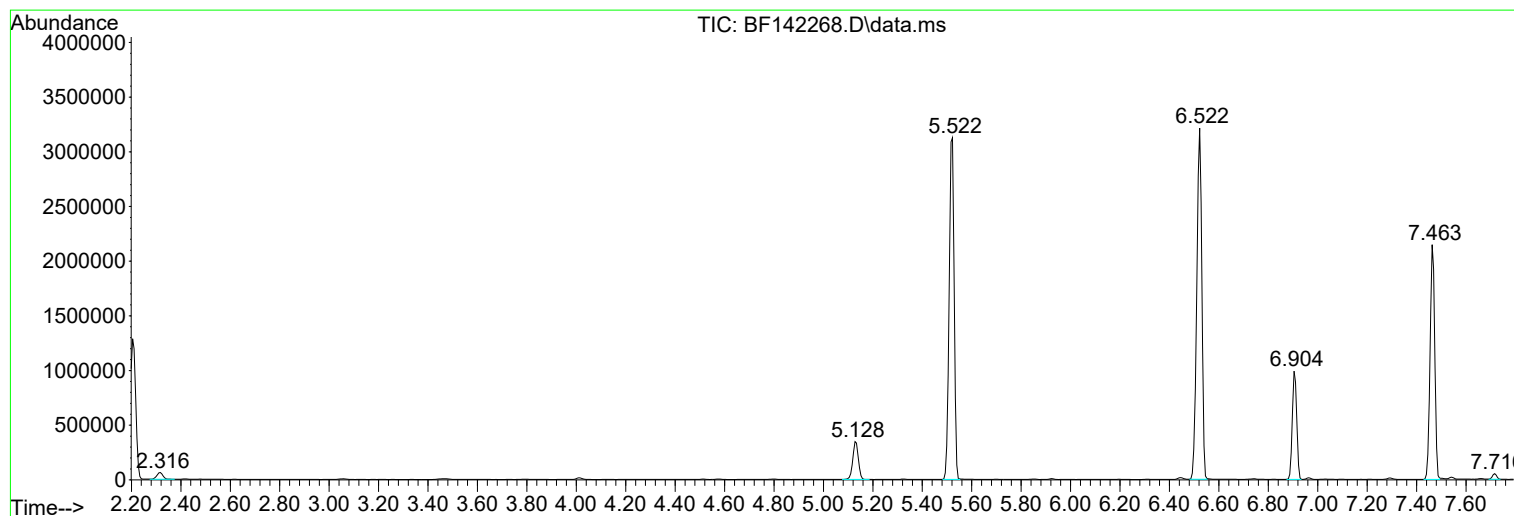
Sum of corrected areas: 36150746

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050125\
Data File : BF142268.D
Acq On : 01 May 2025 18:55
Operator : RC/JU
Sample : Q1901-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-167-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043025.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_F\Data\BF050125\
Data File : BF142268.D
Acq On : 01 May 2025 18:55
Operator : RC/JU
Sample : Q1901-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-167-SB01

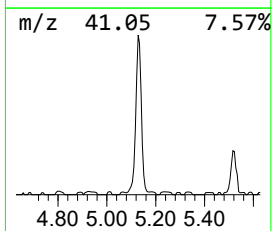
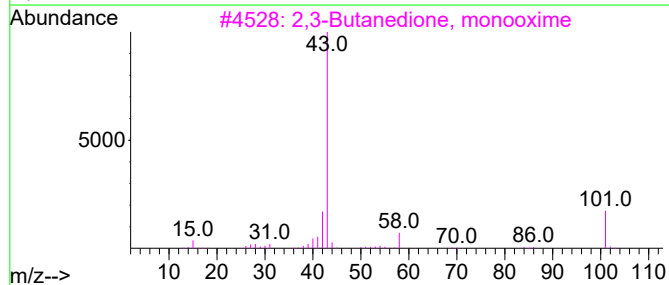
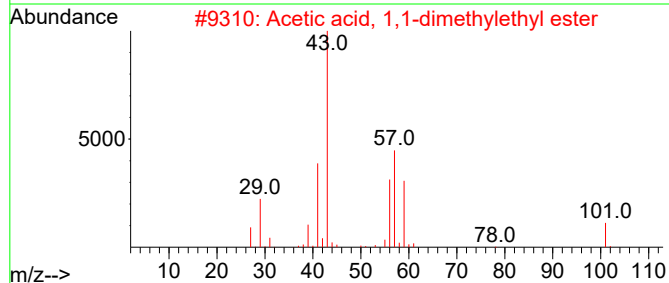
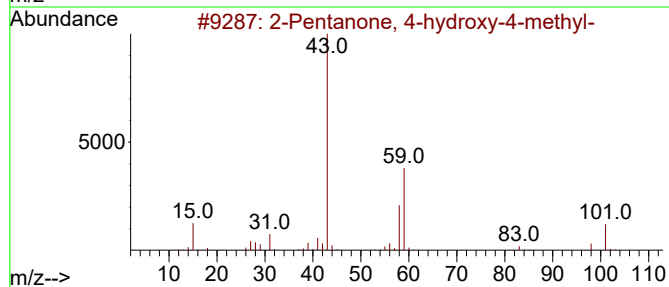
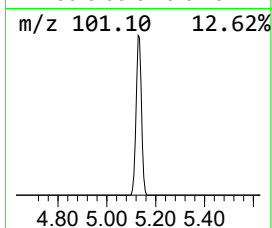
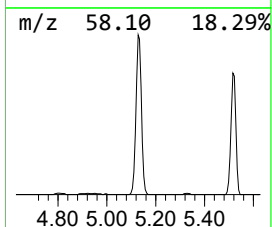
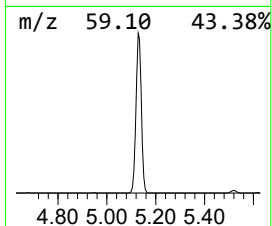
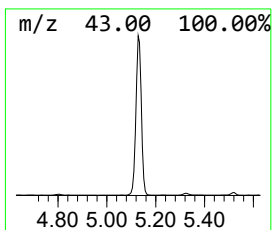
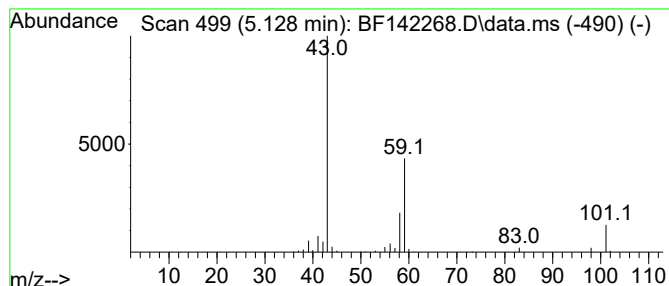
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.128	8.95 ng	542647	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	83		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050125\
Data File : BF142268.D
Acq On : 01 May 2025 18:55
Operator : RC/JU
Sample : Q1901-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-167-SB01

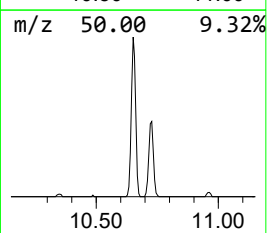
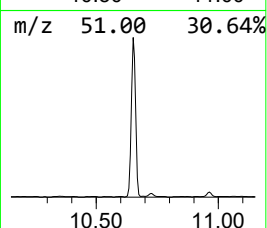
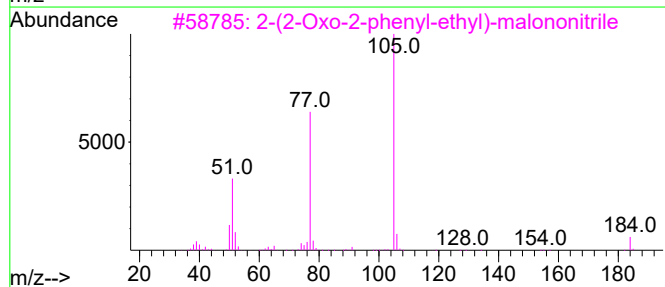
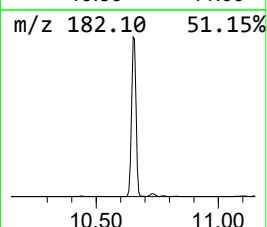
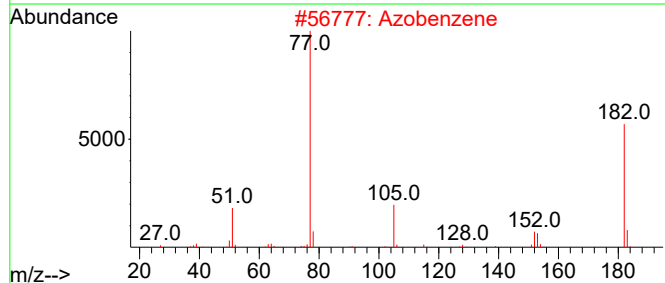
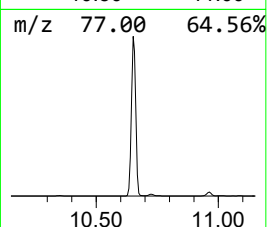
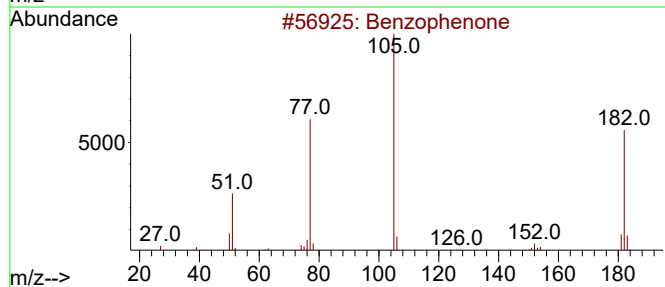
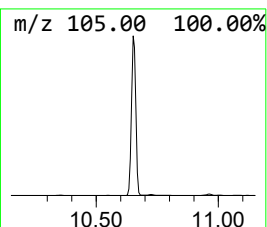
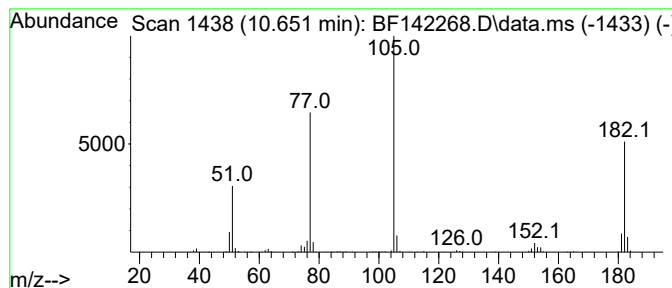
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.651	9.42 ng	733968	Acenaphthene-d10	9.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	58
3			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	58
4			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	52
5			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050125\
Data File : BF142268.D
Acq On : 01 May 2025 18:55
Operator : RC/JU
Sample : Q1901-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-167-SB01

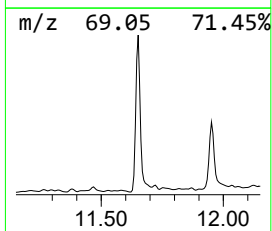
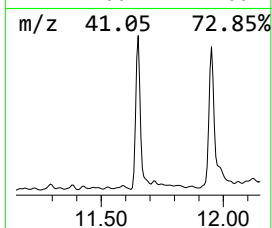
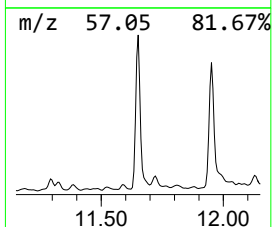
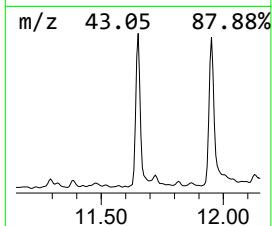
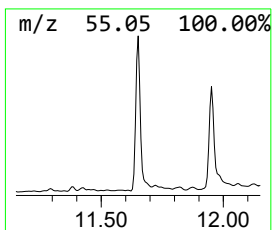
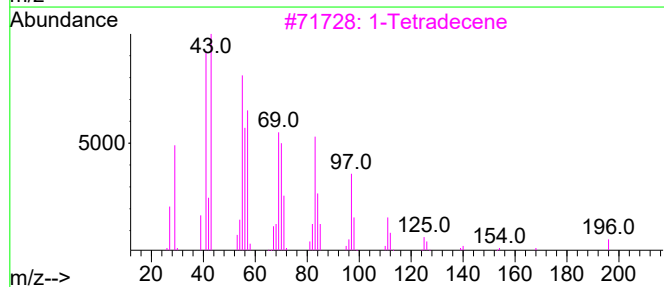
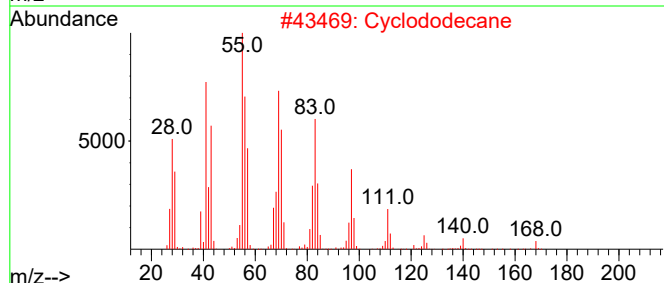
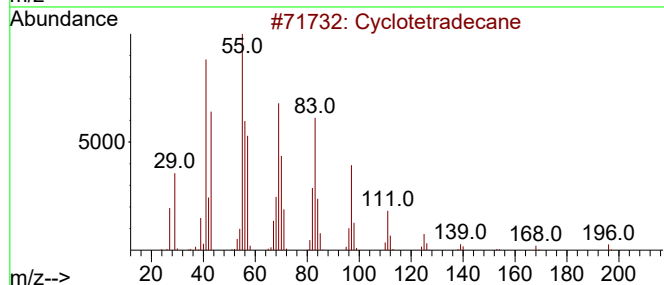
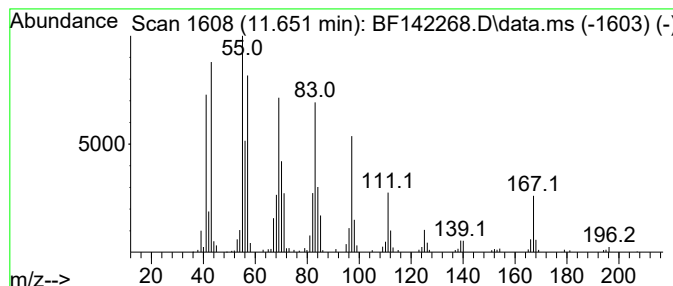
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Cyclotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.651	3.30 ng	241763	Phenanthrene-d10	11.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetradecane	196	C14H28	000295-17-0	96
2			Cyclododecane	168	C12H24	000294-62-2	96
3			1-Tetradecene	196	C14H28	001120-36-1	95
4			1-Hexadecanol	242	C16H34O	036653-82-4	93
5			5-Tetradecene, (Z)-	196	C14H28	041446-62-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050125\
Data File : BF142268.D
Acq On : 01 May 2025 18:55
Operator : RC/JU
Sample : Q1901-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-167-SB01

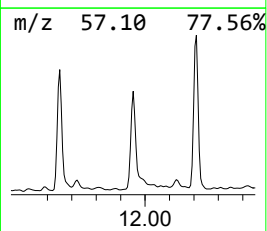
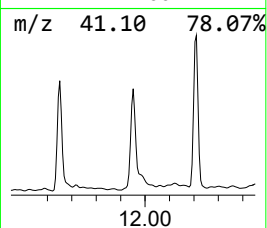
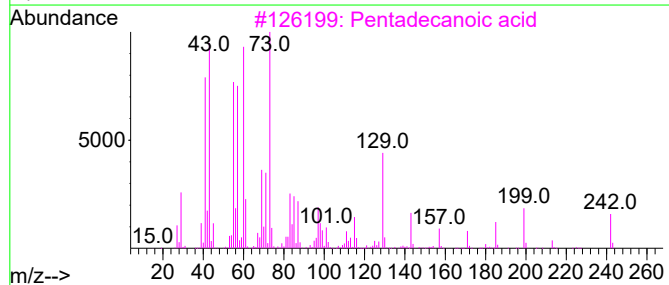
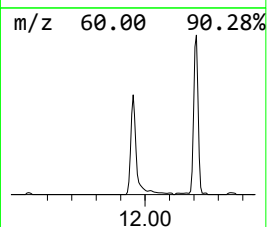
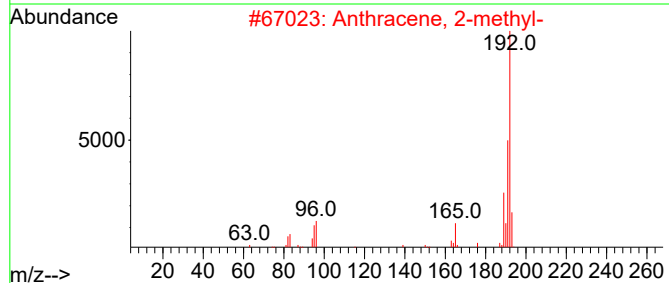
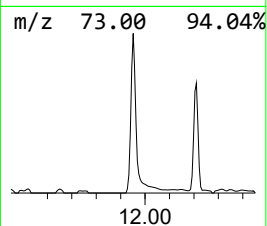
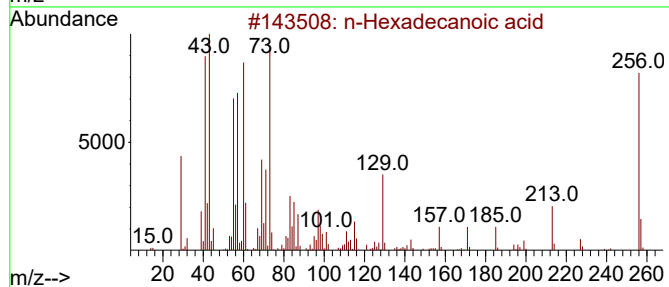
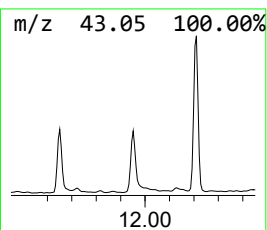
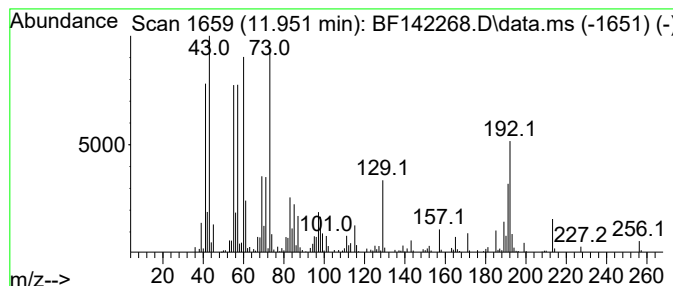
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	4.09 ng	300023	Phenanthrene-d10	11.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	56
5			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050125\
Data File : BF142268.D
Acq On : 01 May 2025 18:55
Operator : RC/JU
Sample : Q1901-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-167-SB01

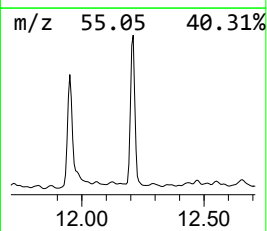
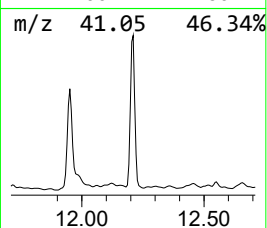
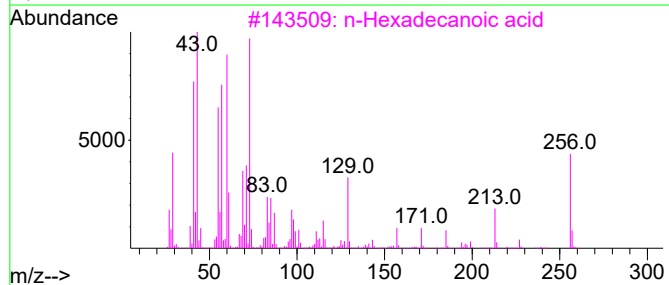
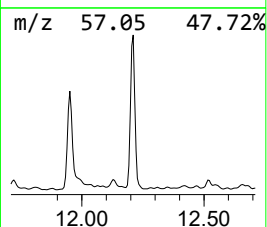
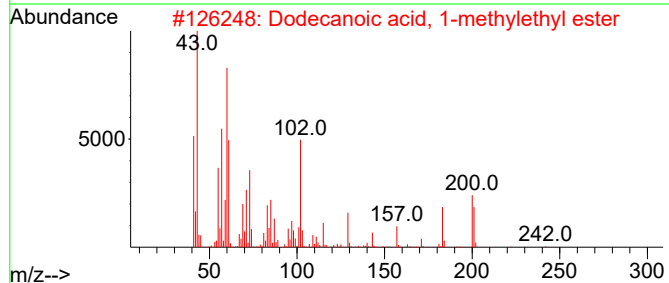
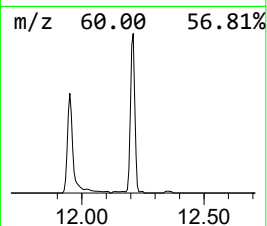
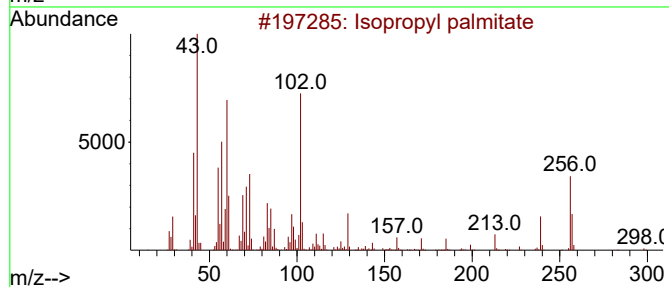
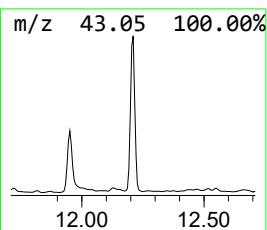
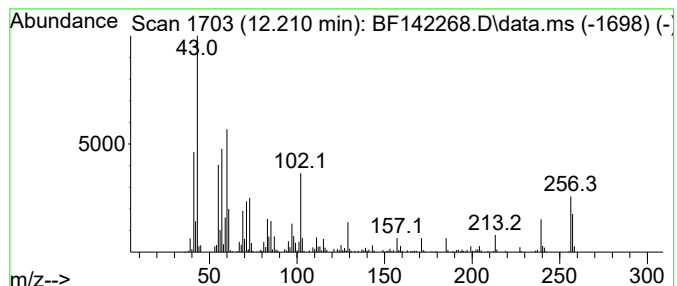
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Isopropyl palmitate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.210	5.47 ng	401290	Phenanthrene-d10	11.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl palmitate	298	C19H38O2	000142-91-6	91
2			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	64
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
4			n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	50
5			8-Methylnonanoic acid, isopropyl...	214	C13H26O2	1000452-00-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050125\
Data File : BF142268.D
Acq On : 01 May 2025 18:55
Operator : RC/JU
Sample : Q1901-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-167-SB01

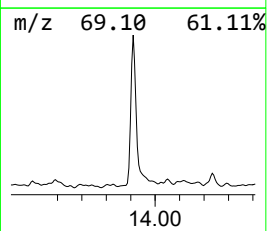
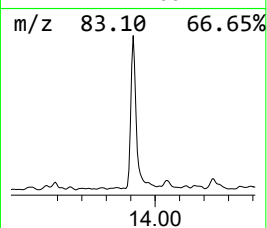
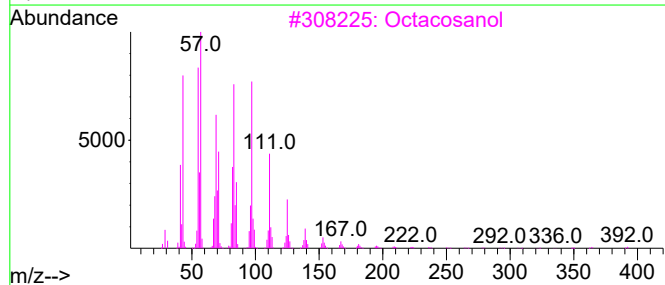
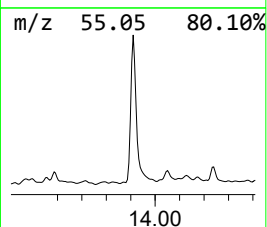
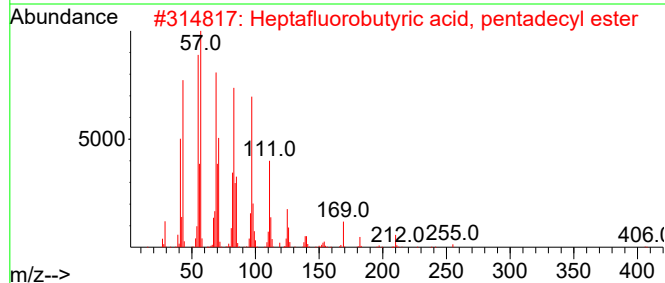
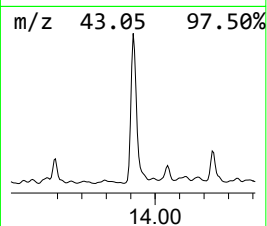
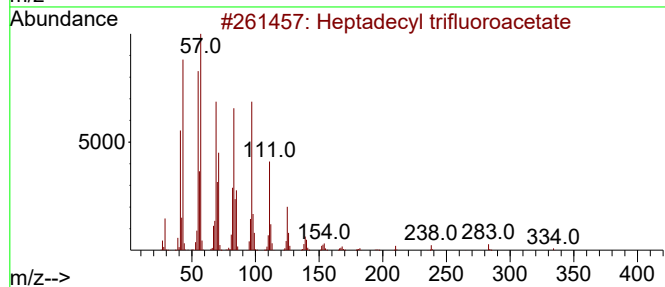
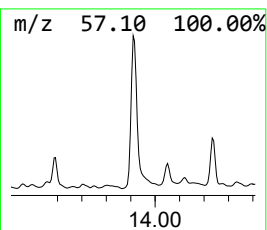
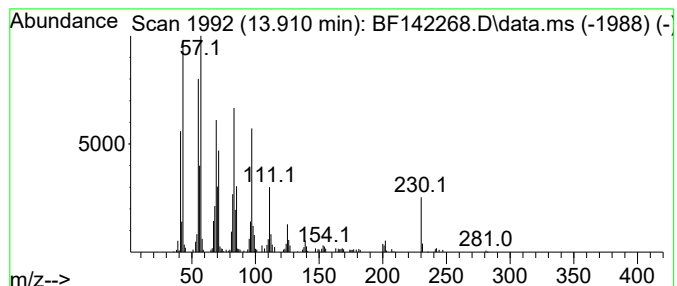
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	2.98 ng	230126	Chrysene-d12	14.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	93
2			Heptafluorobutyric acid, pentadecyl ester	424	C19H31F7O2	959261-23-5	93
3			Octacosanol	410	C28H58O	000557-61-9	93
4			Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	90
5			1-Hexacosene	364	C26H52	018835-33-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050125\
Data File : BF142268.D
Acq On : 01 May 2025 18:55
Operator : RC/JU
Sample : Q1901-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-167-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043025.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-...	5.128	8.9	ng	542647	1	6.904	1212300	20.0
Benzophenone	10.651	9.4	ng	733968	3	9.939	1557660	20.0
Cyclotetradecane	11.651	3.3	ng	241763	4	11.428	1466180	20.0
n-Hexadecanoic ...	11.951	4.1	ng	300023	4	11.428	1466180	20.0
Isopropyl palmi...	12.210	5.5	ng	401290	4	11.428	1466180	20.0
Heptadecyl trif...	13.910	3.0	ng	230126	5	14.069	1542540	20.0