

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122724\
 Data File : BF141004.D
 Acq On : 27 Dec 2024 18:39
 Operator : RC/JU
 Sample : P5382-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-1

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-BF122624.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141004.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.051	498	503	511	rVB	48437	82329	1.05%	0.141%
2	5.434	561	568	573	rBV	4792366	6552705	83.89%	11.215%
3	6.439	732	739	745	rBV	4545741	6769524	86.67%	11.586%
4	6.822	799	804	809	rBV	1220751	1484135	19.00%	2.540%
5	7.381	893	899	905	rBV	3161992	4360604	55.83%	7.463%
6	7.639	938	943	948	rBV	130184	156880	2.01%	0.269%
7	8.104	1016	1022	1027	rBV	1612733	2039678	26.11%	3.491%
8	9.180	1198	1205	1210	rBV	5875453	7811099	100.00%	13.369%
9	9.857	1314	1320	1324	rBV	1802217	2328053	29.80%	3.985%
10	10.569	1436	1441	1446	rVB	712106	882376	11.30%	1.510%
11	10.639	1447	1453	1469	rBV	3767581	5074064	64.96%	8.685%
12	11.339	1567	1572	1580	rBV2	1825362	2967102	37.99%	5.078%
13	11.410	1580	1584	1588	rVB	116053	149992	1.92%	0.257%
14	11.569	1605	1611	1620	rBV3	76699	145317	1.86%	0.249%
15	11.839	1653	1657	1658	rBV	79073	84842	1.09%	0.145%
16	11.874	1658	1663	1668	rVV2	840939	1243434	15.92%	2.128%
17	11.951	1672	1676	1684	rVB	130545	272150	3.48%	0.466%
18	12.133	1702	1707	1715	rVB3	105071	198352	2.54%	0.339%
19	12.551	1773	1778	1784	rBV	696936	882618	11.30%	1.511%
20	12.657	1791	1796	1802	rBV	148433	239739	3.07%	0.410%
21	12.774	1808	1816	1822	rBV	544764	875062	11.20%	1.498%
22	12.927	1833	1842	1847	rBV	5466833	7162469	91.70%	12.259%
23	12.998	1850	1854	1861	rVB5	43092	79928	1.02%	0.137%
24	13.104	1862	1872	1876	rBV3	81830	160310	2.05%	0.274%
25	13.827	1991	1995	2004	rVB2	344250	526357	6.74%	0.901%
26	13.974	2013	2020	2032	rBV2	1375685	2284894	29.25%	3.911%
27	14.745	2147	2151	2161	rBV3	134143	284661	3.64%	0.487%
28	15.010	2191	2196	2205	rBV	274937	602510	7.71%	1.031%
29	15.110	2210	2213	2222	rVB2	72938	116319	1.49%	0.199%
30	15.304	2242	2246	2252	rVB	136692	210687	2.70%	0.361%
31	15.368	2252	2257	2262	rVB	213673	314004	4.02%	0.537%
32	15.433	2262	2268	2281	rBV	956990	1596843	20.44%	2.733%
33	15.974	2355	2360	2370	rVB5	50302	108098	1.38%	0.185%
34	16.868	2506	2512	2521	rVB2	90215	212644	2.72%	0.364%
35	17.298	2580	2585	2600	rVB	68769	166242	2.13%	0.285%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122724\
Data File : BF141004.D
Acq On : 27 Dec 2024 18:39
Operator : RC/JU
Sample : P5382-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

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-BF122624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

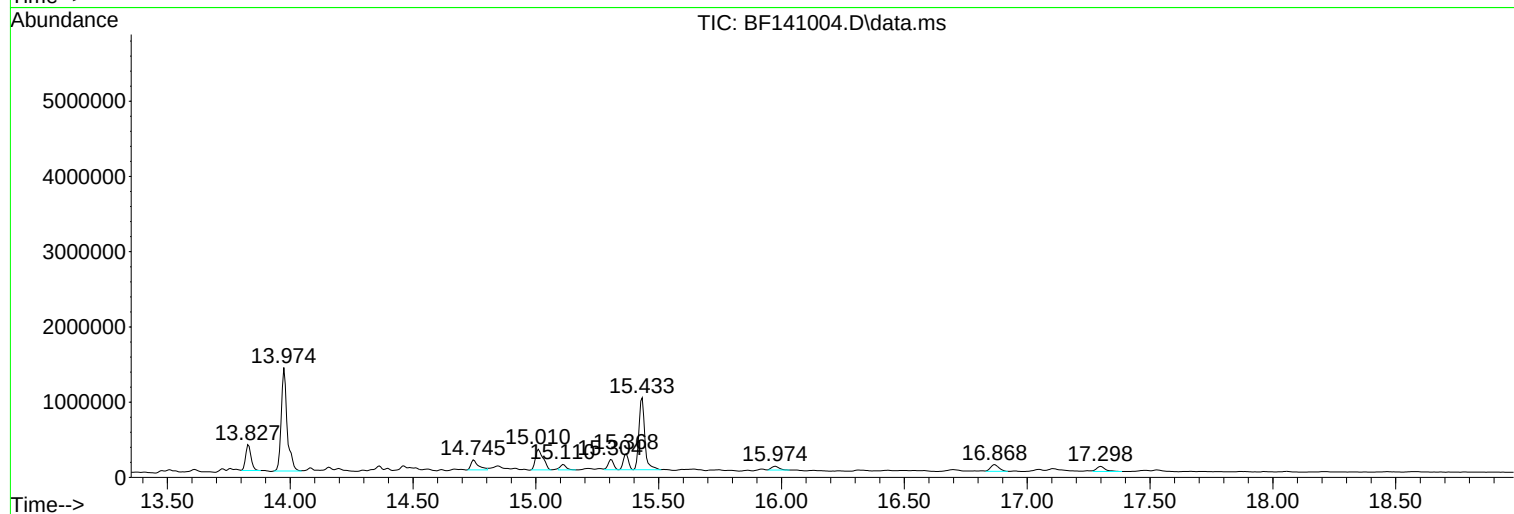
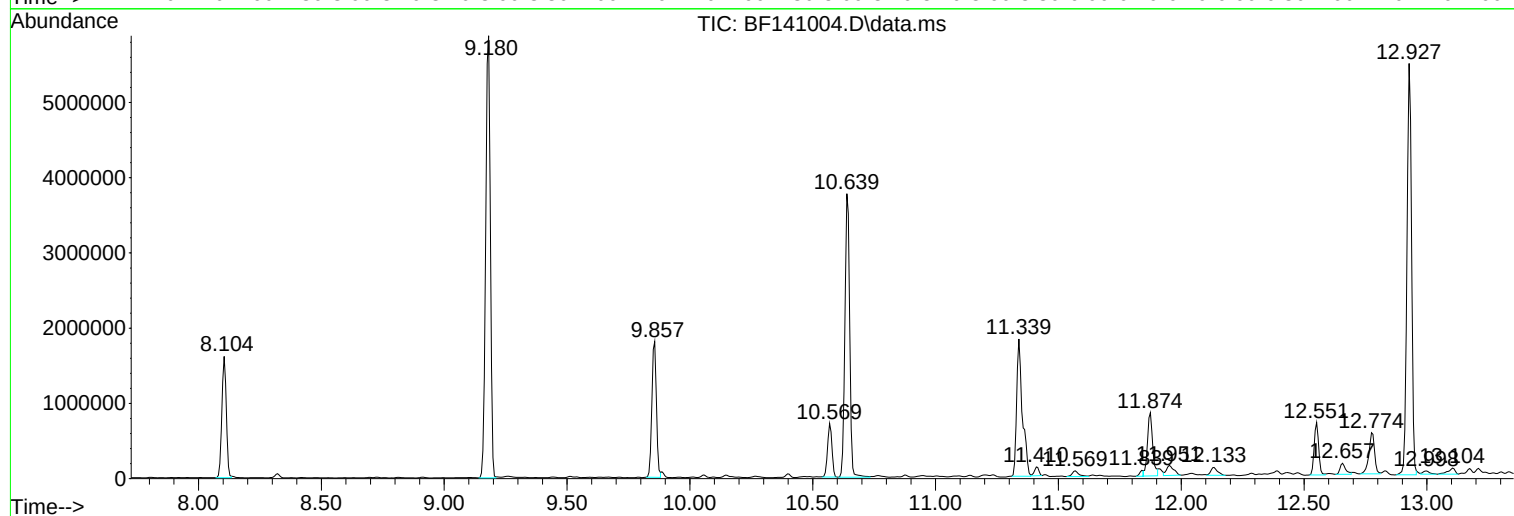
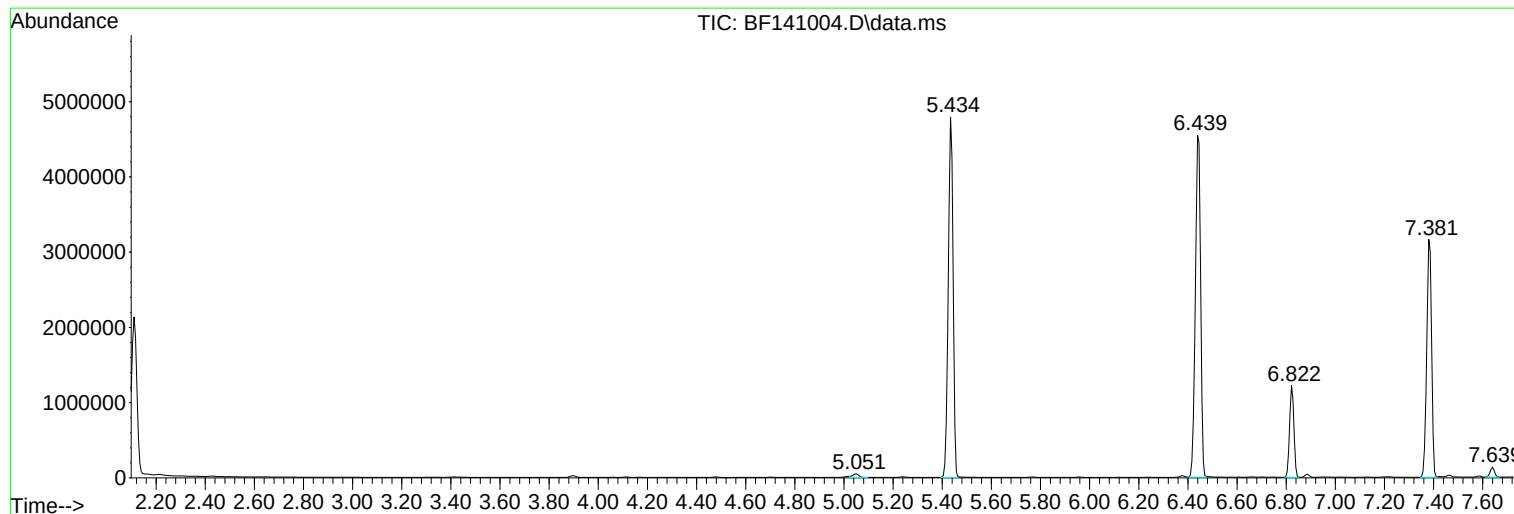
Sum of corrected areas: 58426021

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122724\
Data File : BF141004.D
Acq On : 27 Dec 2024 18:39
Operator : RC/JU
Sample : P5382-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.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\BF122724\
Data File : BF141004.D
Acq On : 27 Dec 2024 18:39
Operator : RC/JU
Sample : P5382-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

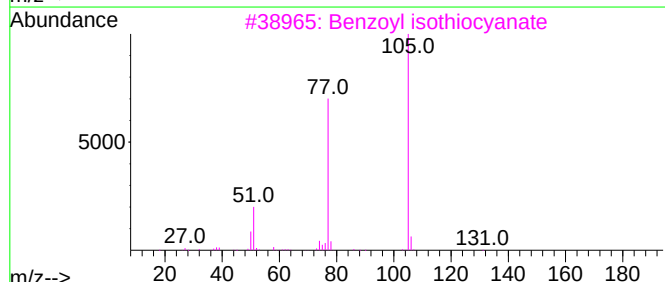
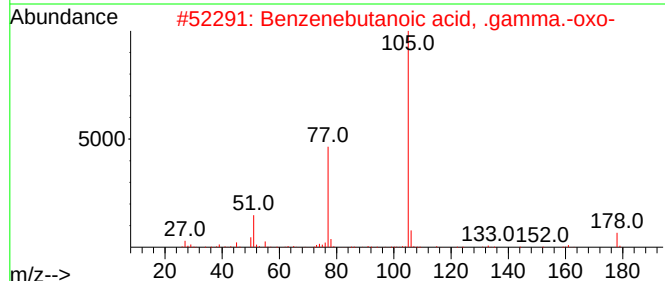
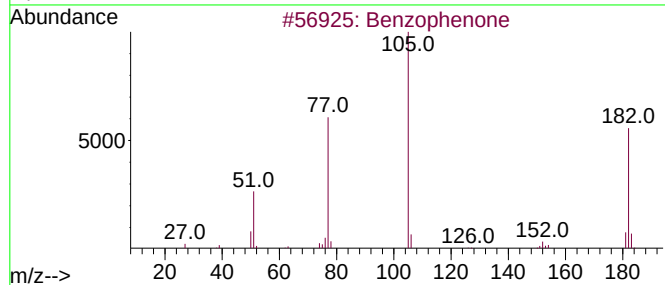
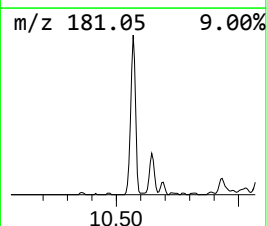
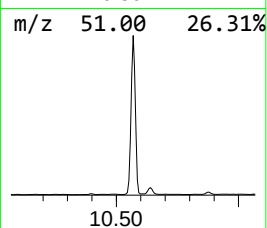
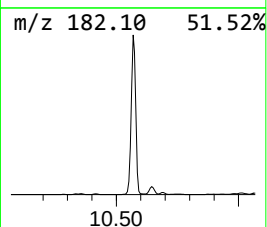
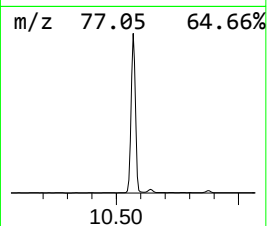
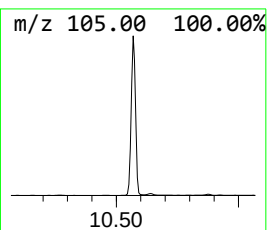
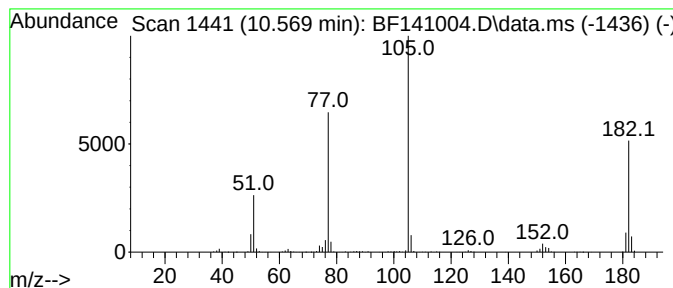
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.569	7.58 ng	882376	Acenaphthene-d10	9.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
3			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
4			Vinyl benzoate	148	C9H8O2	000769-78-8	47
5			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122724\
Data File : BF141004.D
Acq On : 27 Dec 2024 18:39
Operator : RC/JU
Sample : P5382-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

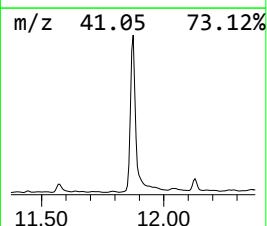
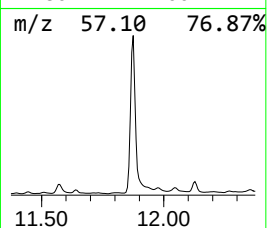
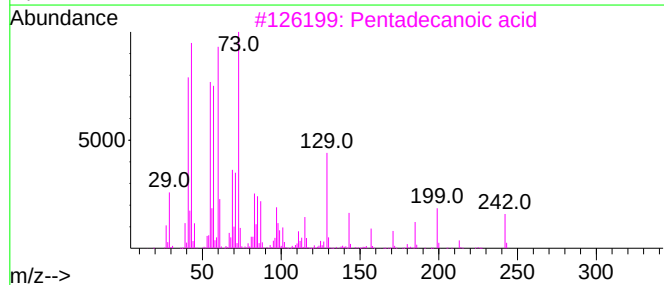
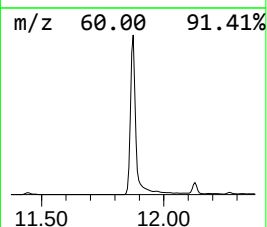
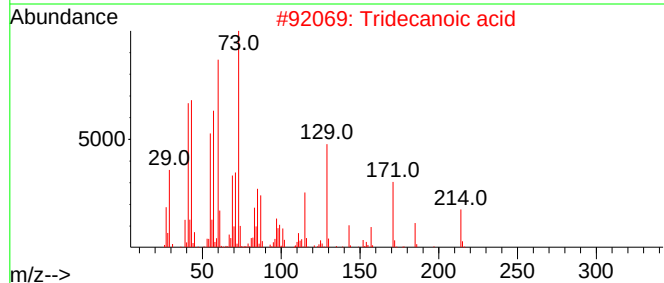
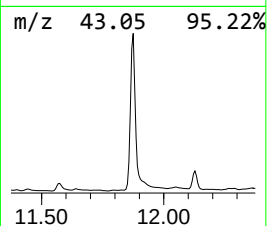
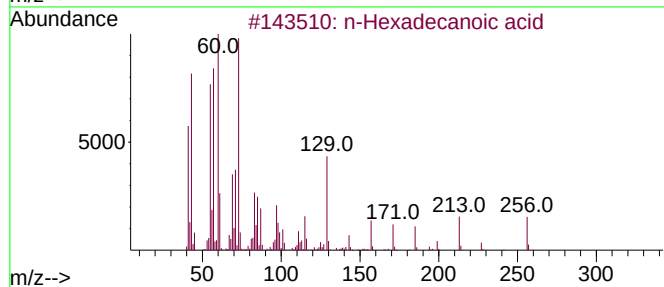
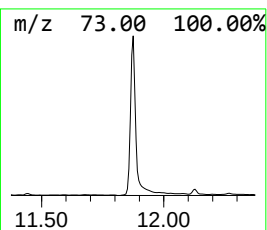
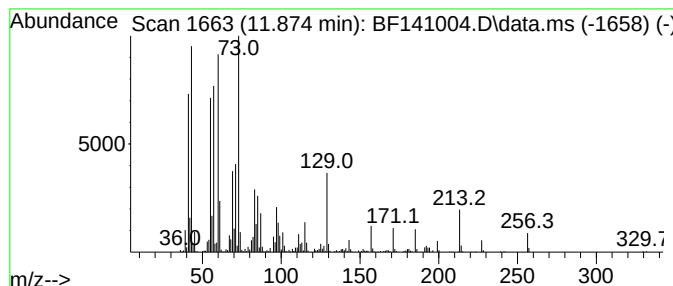
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.874	8.38 ng	1243430	Phenanthrene-d10	11.339

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	92
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122724\
Data File : BF141004.D
Acq On : 27 Dec 2024 18:39
Operator : RC/JU
Sample : P5382-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

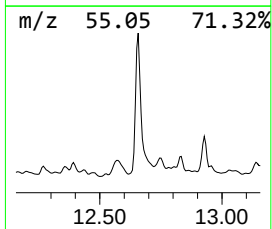
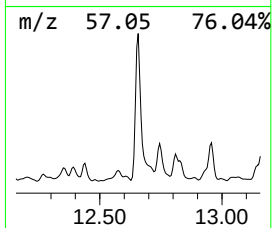
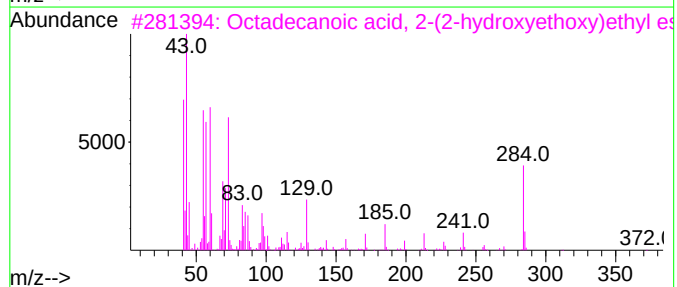
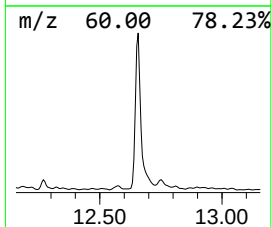
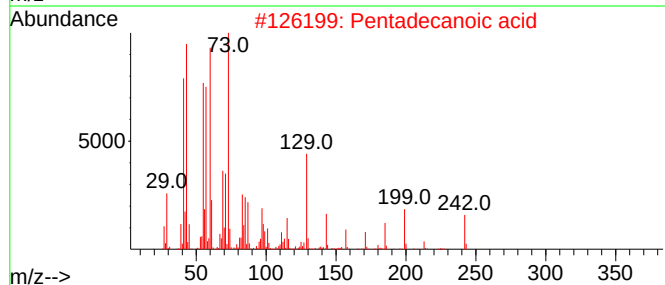
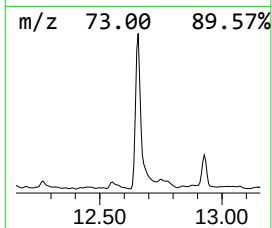
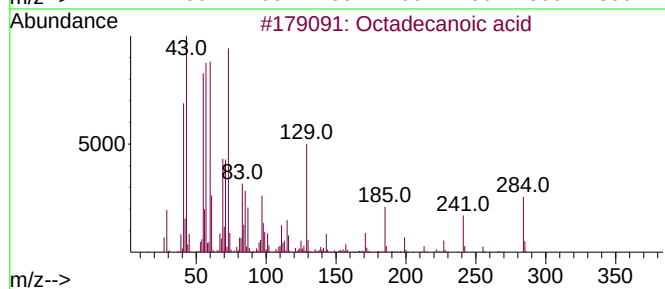
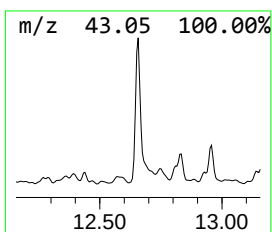
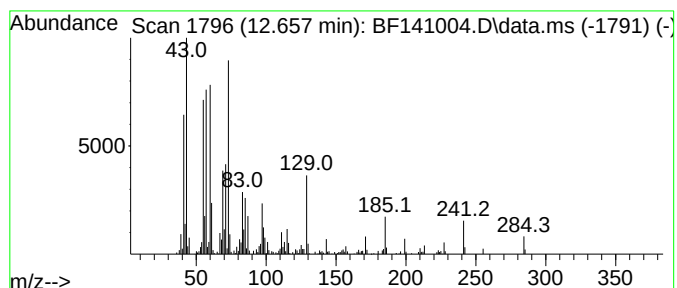
Instrument :
BNA_F
ClientSampleId :
COMP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.657	2.10 ng	239739	Chrysene-d12	13.974	
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	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122724\
Data File : BF141004.D
Acq On : 27 Dec 2024 18:39
Operator : RC/JU
Sample : P5382-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

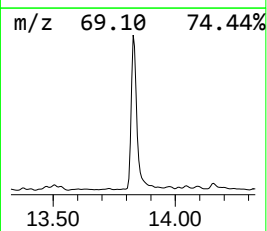
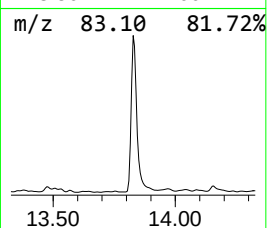
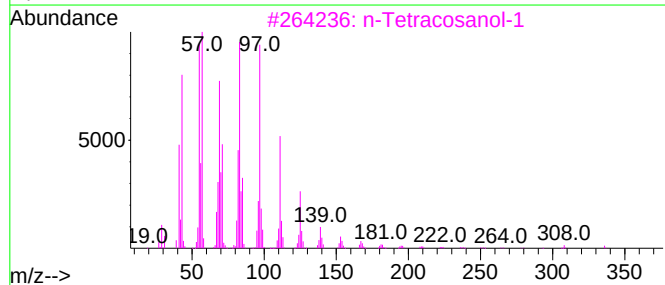
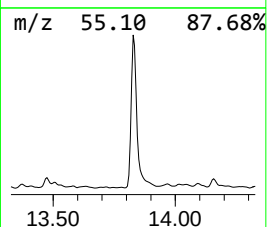
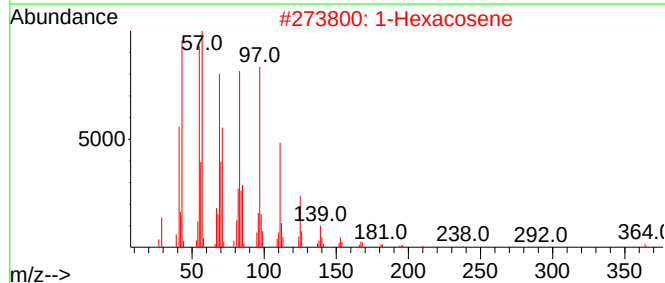
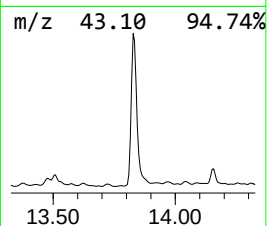
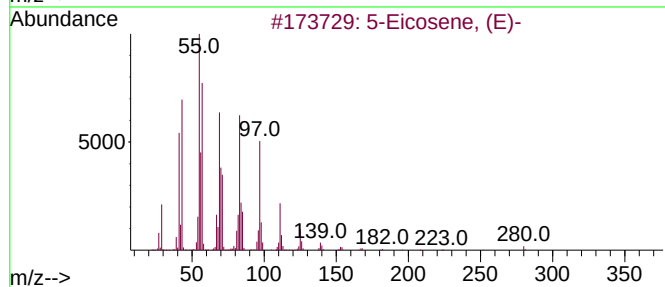
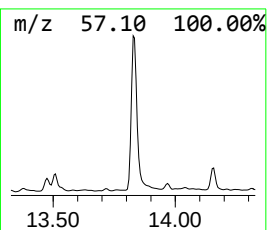
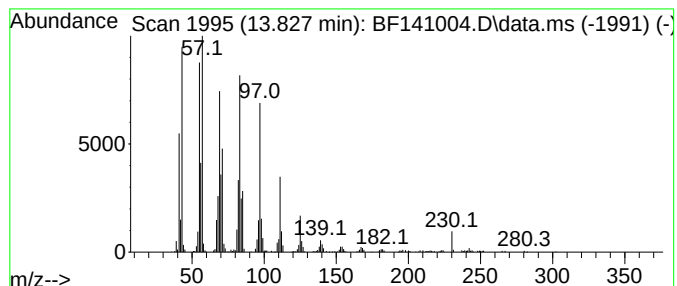
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	4.61 ng	526357	Chrysene-d12	13.974

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2		1-Hexacosene	364	C26H52	018835-33-1	94
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4		2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91
5		2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122724\
Data File : BF141004.D
Acq On : 27 Dec 2024 18:39
Operator : RC/JU
Sample : P5382-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

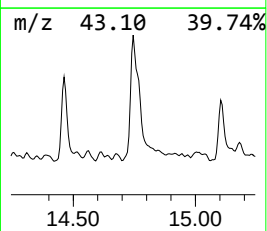
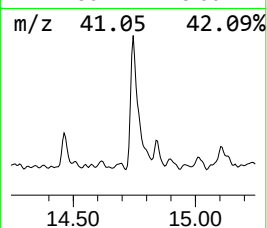
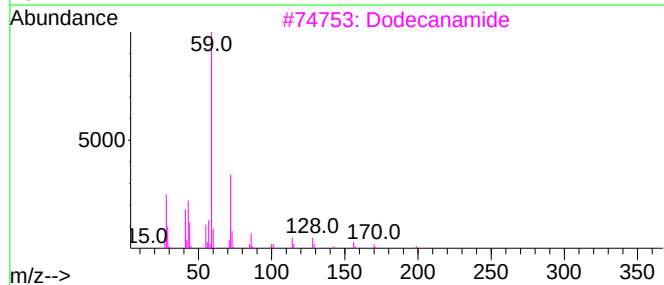
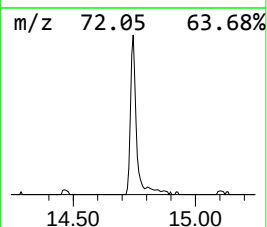
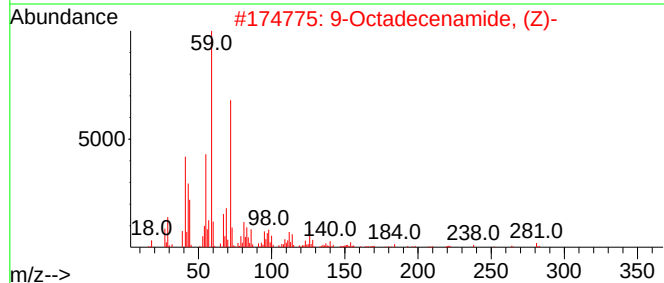
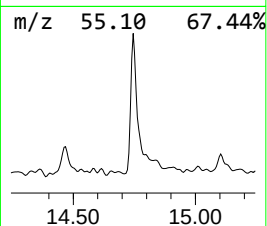
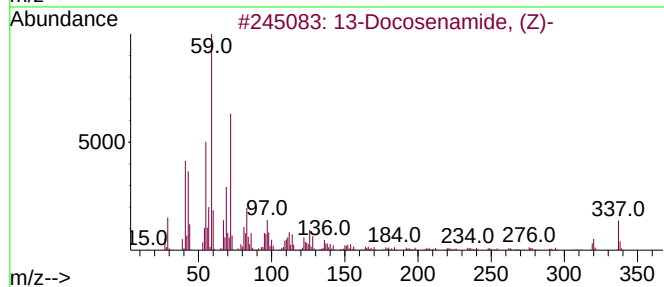
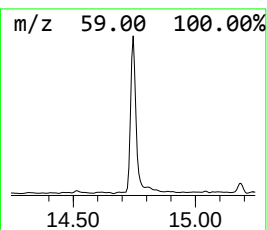
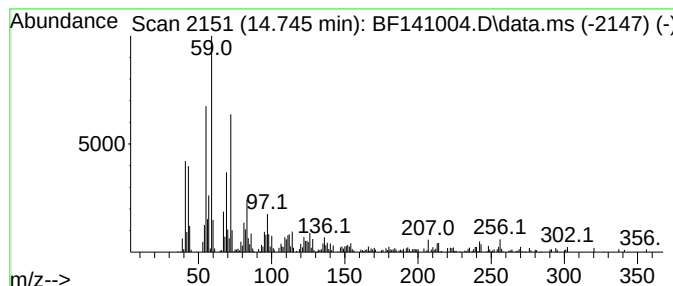
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.745	3.57 ng	284661	Perylene-d12	15.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3			Dodecanamide	199	C12H25NO	001120-16-7	64
4			Palmitoleamide	253	C16H31NO	106010-22-4	58
5			Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122724\
Data File : BF141004.D
Acq On : 27 Dec 2024 18:39
Operator : RC/JU
Sample : P5382-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

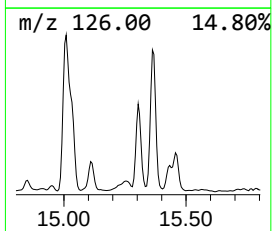
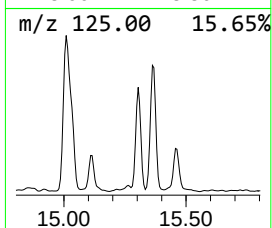
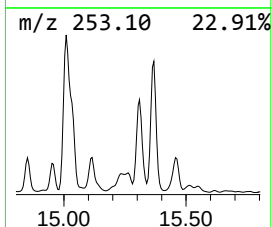
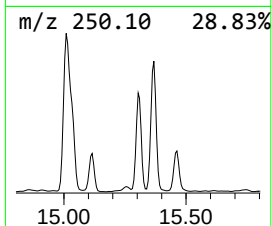
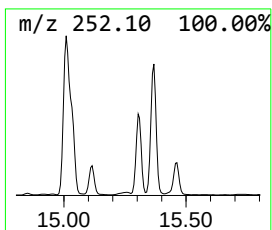
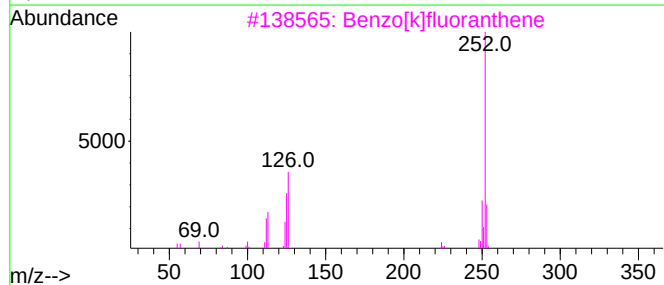
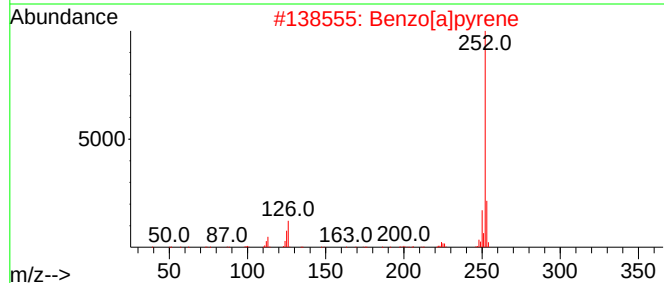
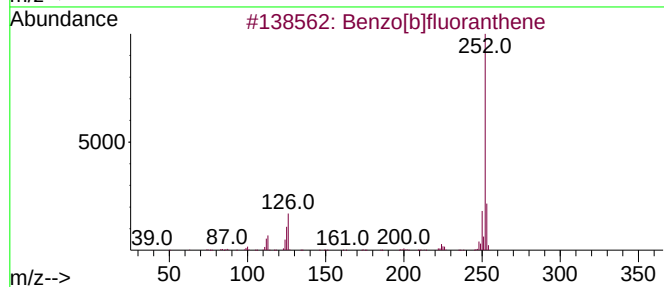
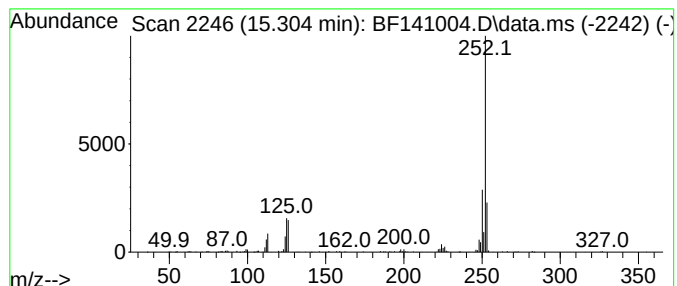
Instrument :
BNA_F
ClientSampleId :
COMP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.304	2.64 ng	210687	Perylene-d12	15.433	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4	Benzo[e]pyrene	252	C20H12	000192-97-2	94
5	Perylene	252	C20H12	000198-55-0	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122724\
Data File : BF141004.D
Acq On : 27 Dec 2024 18:39
Operator : RC/JU
Sample : P5382-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.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
Benzophenone	10.569	7.6	ng	882376	3	9.857	2328050	20.0
n-Hexadecanoic ...	11.874	8.4	ng	1243430	4	11.339	2967100	20.0
Octadecanoic acid	12.657	2.1	ng	239739	5	13.974	2284890	20.0
5-Eicosene, (E)-	13.827	4.6	ng	526357	5	13.974	2284890	20.0
13-Docosenamide...	14.745	3.6	ng	284661	6	15.433	1596840	20.0
Benzo[e]pyrene	15.304	2.6	ng	210687	6	15.433	1596840	20.0