

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022125\
 Data File : BF141723.D
 Acq On : 21 Feb 2025 16:47
 Operator : RC/JU
 Sample : Q1388-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-12016

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-BF020625.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141723.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.399	557	562	589	rBV	1387288	1965325	81.14%	11.072%
2	6.416	730	735	764	rBV	1371839	2037209	84.11%	11.477%
3	6.775	791	796	806	rBV	423144	549640	22.69%	3.096%
4	7.340	887	892	904	rBV	928663	1315918	54.33%	7.413%
5	7.610	932	938	955	rBV	22245	58900	2.43%	0.332%
6	8.063	1009	1015	1034	rBV	500469	751264	31.02%	4.232%
7	9.134	1191	1197	1207	rBV	1892043	2422125	100.00%	13.645%
8	9.216	1207	1211	1221	rVB2	13156	28790	1.19%	0.162%
9	9.810	1307	1312	1316	rBV	629572	816815	33.72%	4.602%
10	10.022	1343	1348	1352	rBV	29885	41782	1.73%	0.235%
11	10.216	1376	1381	1389	rBV	24198	35734	1.48%	0.201%
12	10.363	1401	1406	1411	rBV	46562	61257	2.53%	0.345%
13	10.522	1426	1433	1441	rBV	404985	530256	21.89%	2.987%
14	10.598	1441	1446	1461	rVV	911140	1302669	53.78%	7.339%
15	10.834	1482	1486	1493	rVB	38118	48547	2.00%	0.273%
16	11.298	1560	1565	1575	rBV2	527994	957515	39.53%	5.394%
17	11.375	1575	1578	1585	rVB	18785	26916	1.11%	0.152%
18	11.545	1602	1607	1613	rBV4	21370	57467	2.37%	0.324%
19	11.828	1646	1655	1666	rBV	194504	351062	14.49%	1.978%
20	11.910	1666	1669	1678	rVB2	32067	62411	2.58%	0.352%
21	12.510	1766	1771	1776	rBV	159968	210490	8.69%	1.186%
22	12.610	1784	1788	1794	rBV	27954	50089	2.07%	0.282%
23	12.733	1803	1809	1816	rBV	123518	198328	8.19%	1.117%
24	12.880	1828	1834	1842	rBV	1325858	1715425	70.82%	9.664%
25	13.063	1858	1865	1870	rVB2	15264	31437	1.30%	0.177%
26	13.416	1921	1925	1930	rBV	105672	134627	5.56%	0.758%
27	13.580	1945	1953	1959	rBV2	11502	24779	1.02%	0.140%
28	13.845	1991	1998	2005	rVV7	9126	30440	1.26%	0.171%
29	13.933	2006	2013	2025	rVB2	409443	695797	28.73%	3.920%
30	14.557	2115	2119	2124	rVB	86089	114415	4.72%	0.645%
31	14.645	2130	2134	2137	rBV	39325	57771	2.39%	0.325%
32	14.692	2138	2142	2146	rVV2	36584	63544	2.62%	0.358%
33	14.733	2146	2149	2153	rVB2	35875	46758	1.93%	0.263%
34	14.822	2161	2164	2168	rVB2	33758	45619	1.88%	0.257%
35	14.874	2170	2173	2177	rVB2	35451	49864	2.06%	0.281%
36	14.916	2177	2180	2183	rVB	21374	26913	1.11%	0.152%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022125\
Data File : BF141723.D
Acq On : 21 Feb 2025 16:47
Operator : RC/JU
Sample : Q1388-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12016

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-BF020625.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.963	2183	2188	2195	rBV2	77493	149201	6.16%	0.841%
38	15.257	2233	2238	2243	rVB	37073	57011	2.35%	0.321%
39	15.316	2243	2248	2253	rVV	41720	62322	2.57%	0.351%
40	15.374	2253	2258	2273	rVB	293934	500717	20.67%	2.821%
41	16.810	2497	2502	2508	rBV2	12898	25399	1.05%	0.143%
42	17.239	2570	2575	2590	rVB2	12562	37957	1.57%	0.214%

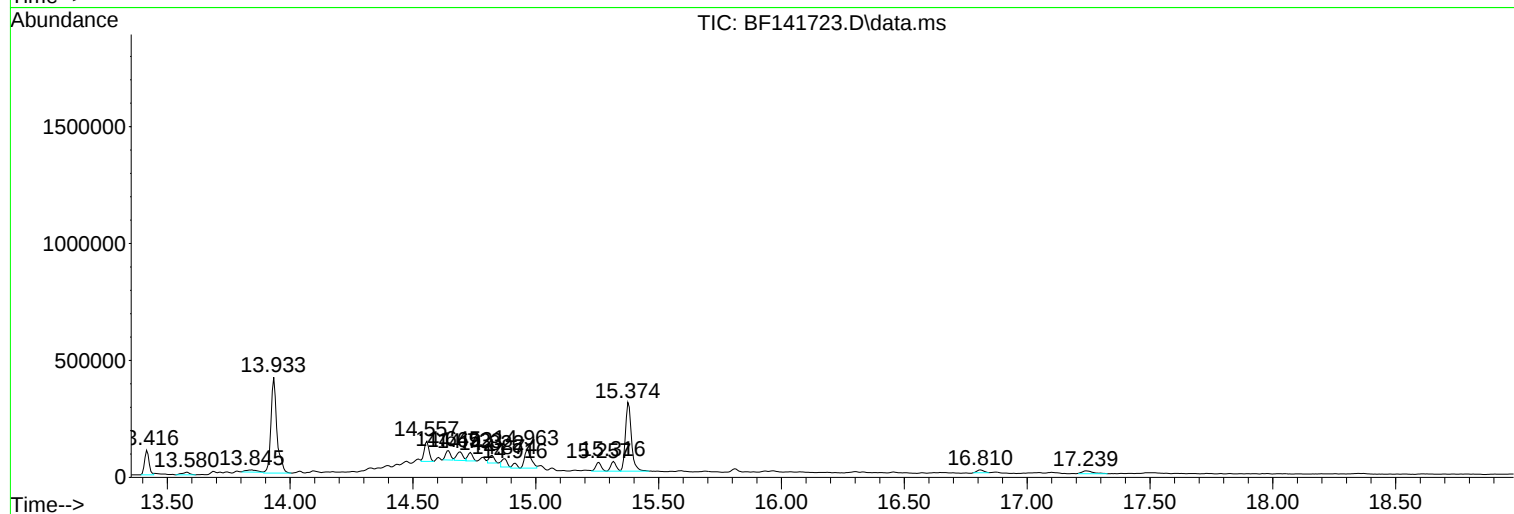
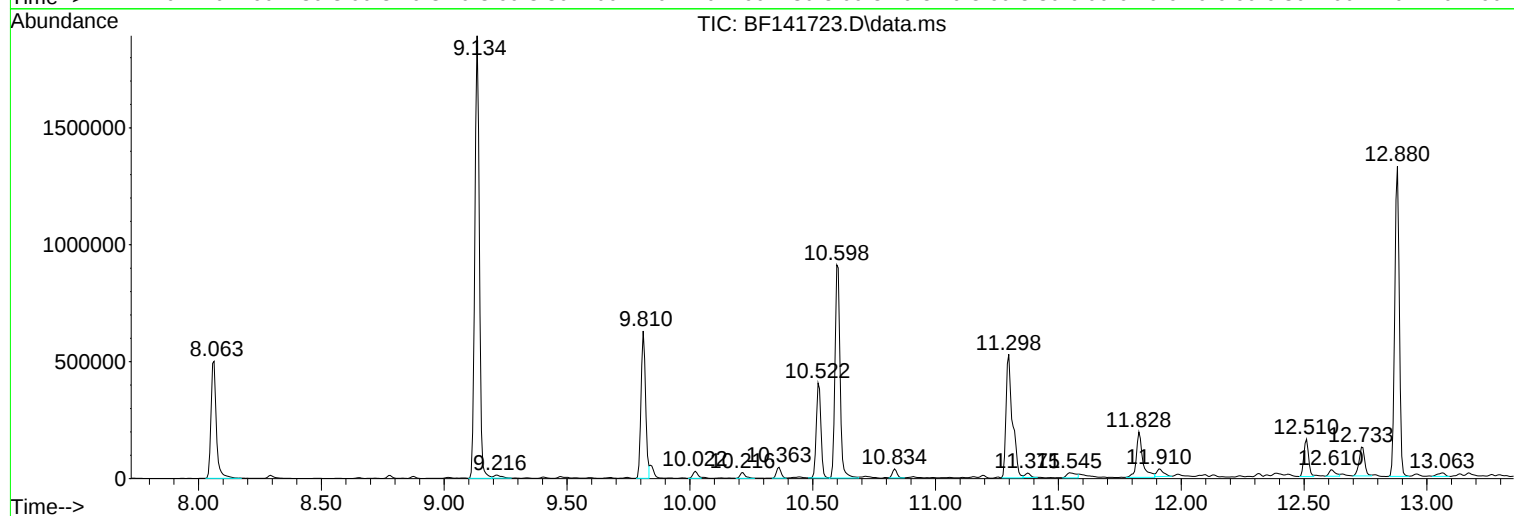
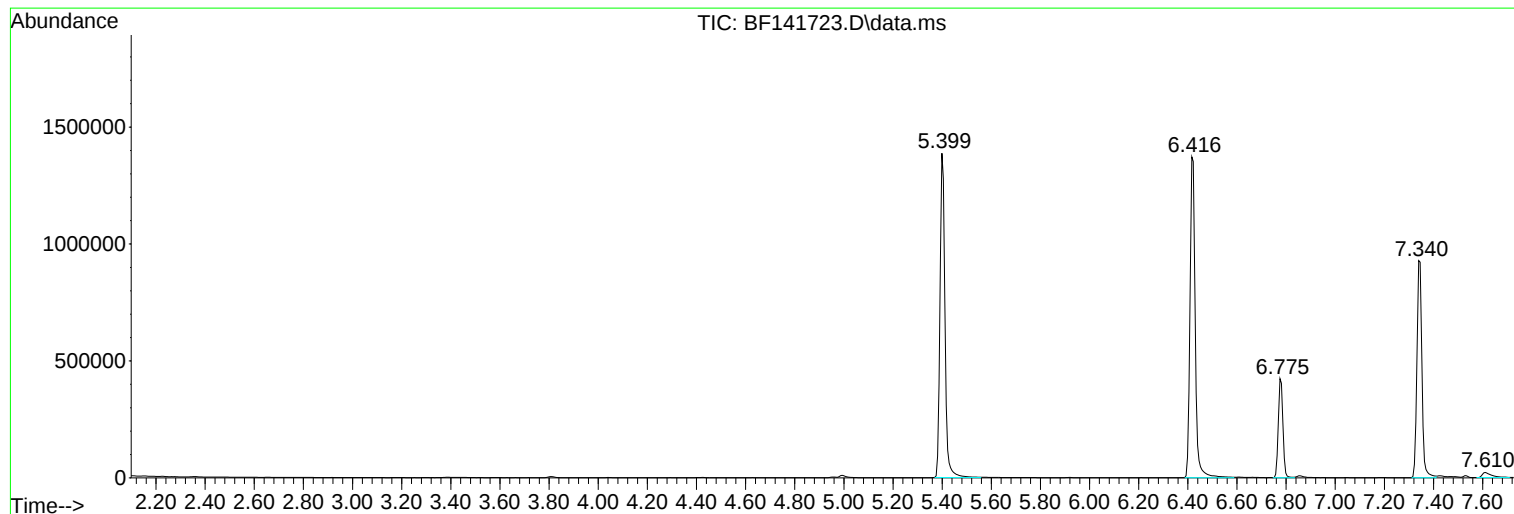
Sum of corrected areas: 17750505

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022125\
Data File : BF141723.D
Acq On : 21 Feb 2025 16:47
Operator : RC/JU
Sample : Q1388-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12016

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.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\BF022125\
Data File : BF141723.D
Acq On : 21 Feb 2025 16:47
Operator : RC/JU
Sample : Q1388-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12016

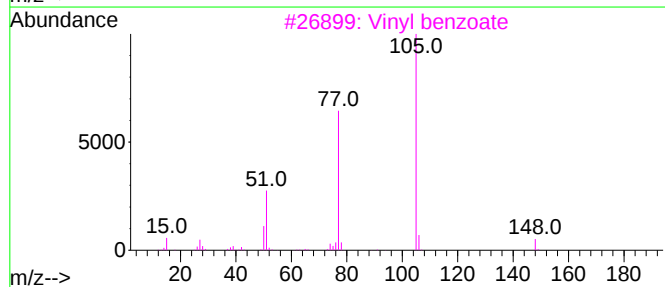
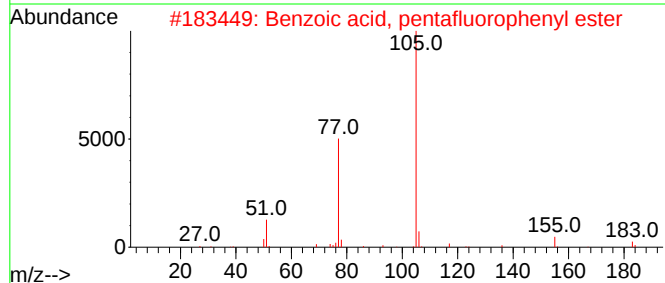
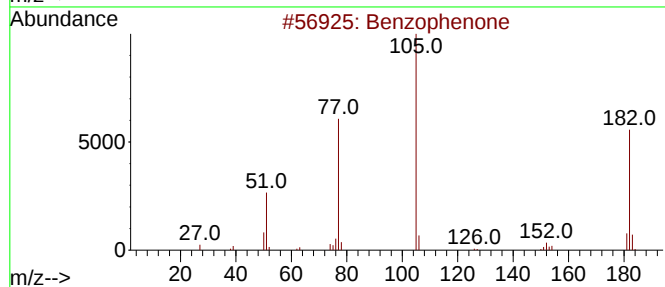
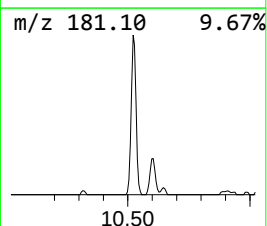
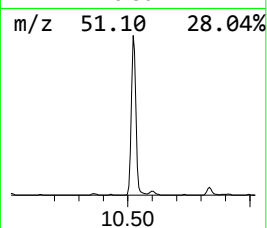
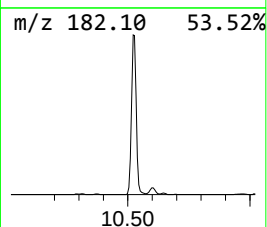
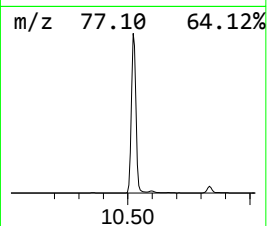
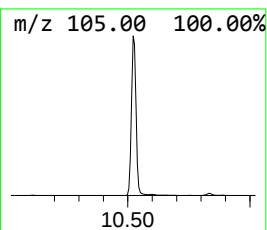
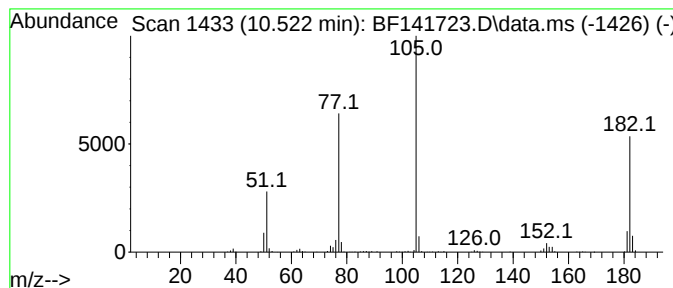
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.522	12.98 ng	530256	Acenaphthene-d10	9.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47
3			Vinyl benzoate	148	C9H8O2	000769-78-8	47
4			Benzilic acid	228	C14H12O3	000076-93-7	47
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022125\
Data File : BF141723.D
Acq On : 21 Feb 2025 16:47
Operator : RC/JU
Sample : Q1388-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12016

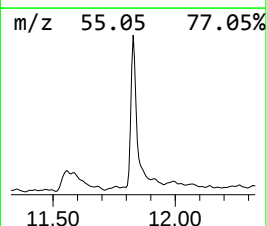
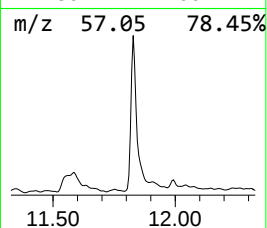
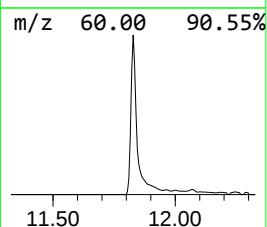
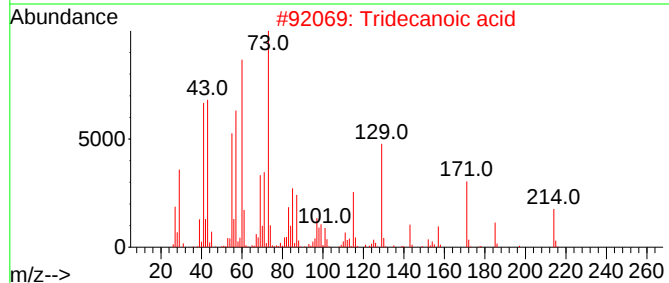
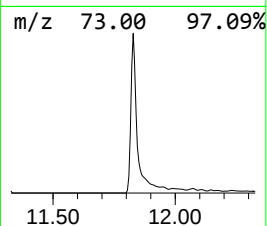
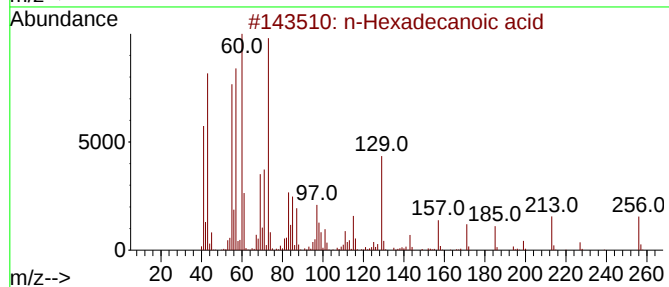
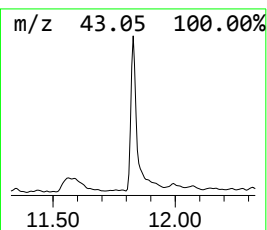
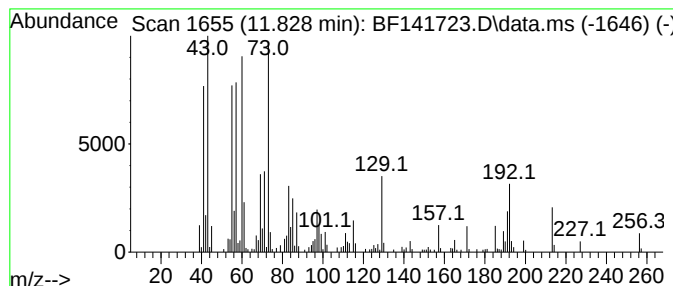
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.828	7.33 ng	351062	Phenanthrene-d10	11.298

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5			Octanoic acid	144	C8H16O2	000124-07-2	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022125\
Data File : BF141723.D
Acq On : 21 Feb 2025 16:47
Operator : RC/JU
Sample : Q1388-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12016

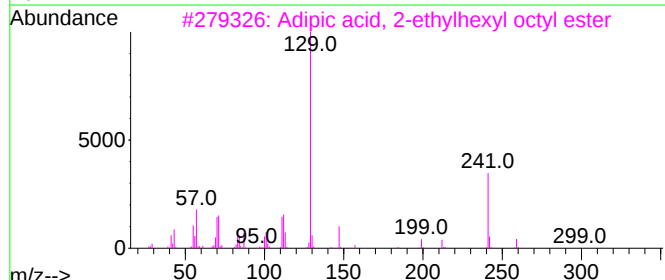
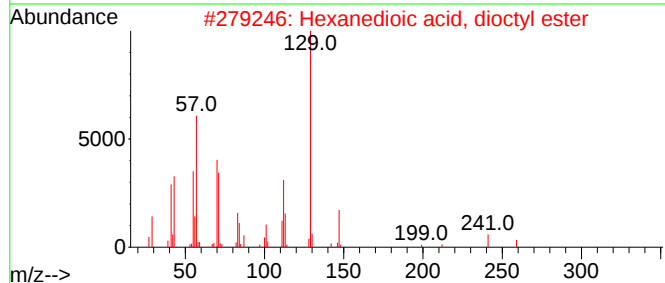
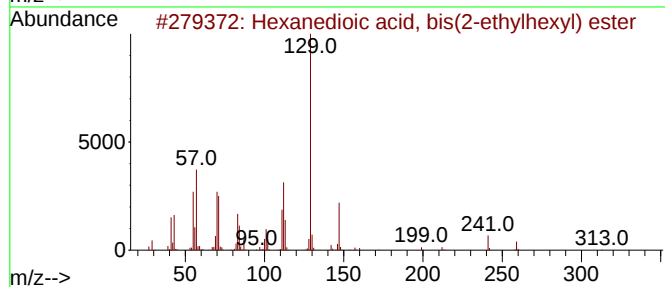
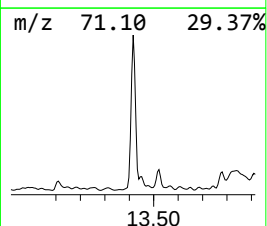
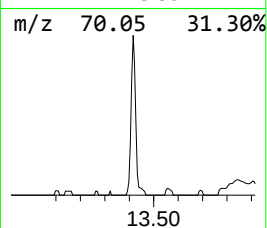
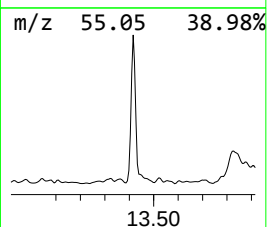
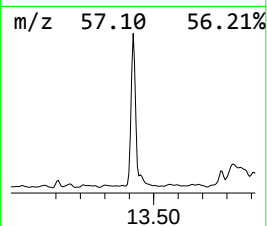
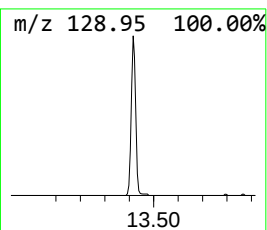
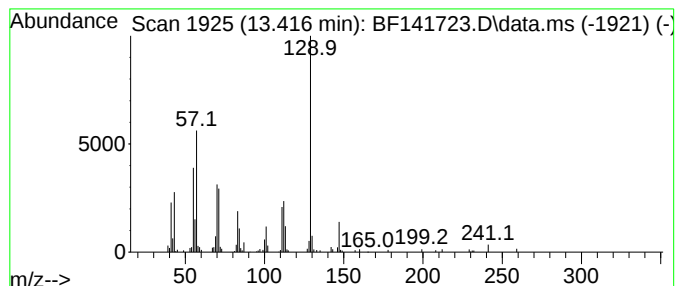
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Hexanedioic acid, bis(2-eth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.416	3.87 ng	134627	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	91
2			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	90
3			Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	83
4			Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	68
5			Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1010324-48-0	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022125\
Data File : BF141723.D
Acq On : 21 Feb 2025 16:47
Operator : RC/JU
Sample : Q1388-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12016

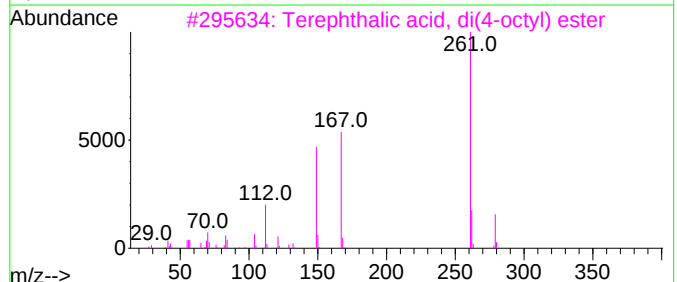
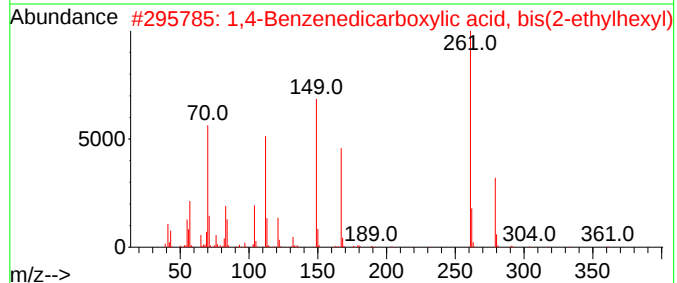
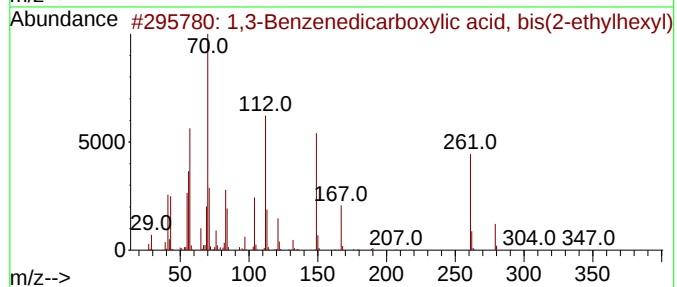
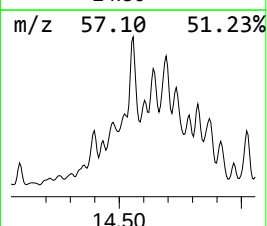
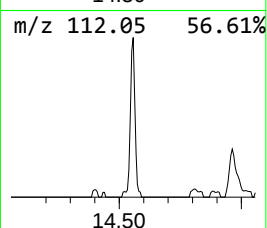
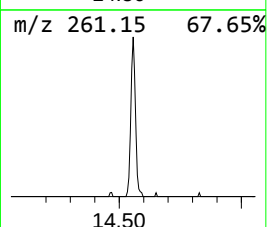
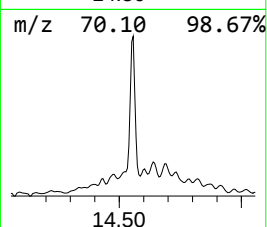
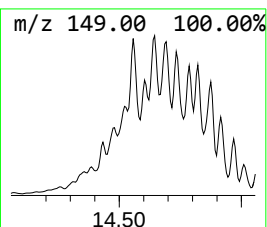
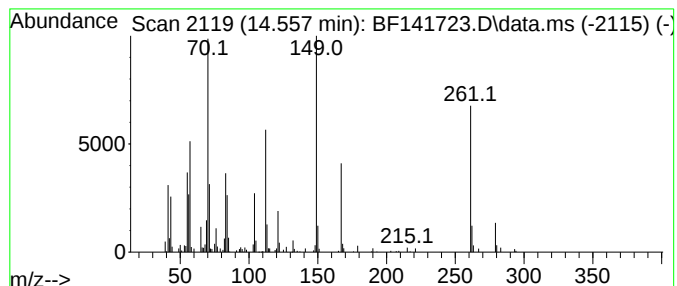
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1,3-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.557	3.29 ng	114415	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	68
2			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	59
3			Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	38
4			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	38
5			Isophthalic acid, 4-methylpent-2...	362	C22H34O4	1000356-44-5	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022125\
Data File : BF141723.D
Acq On : 21 Feb 2025 16:47
Operator : RC/JU
Sample : Q1388-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12016

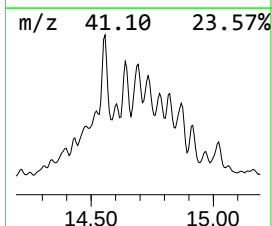
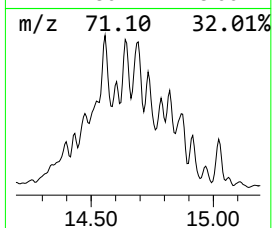
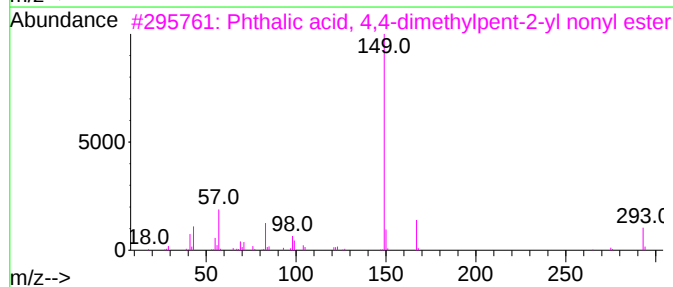
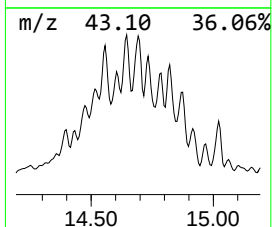
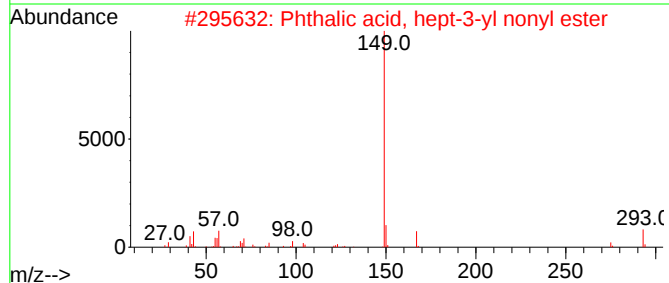
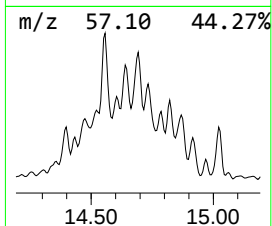
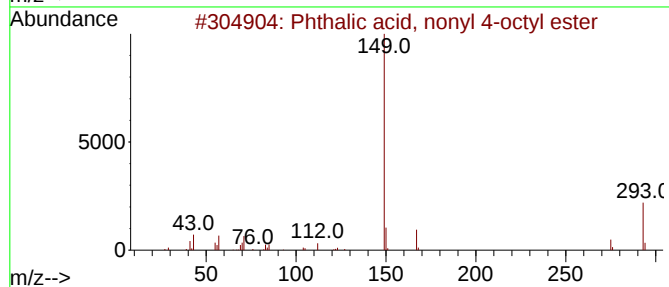
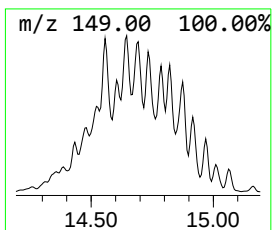
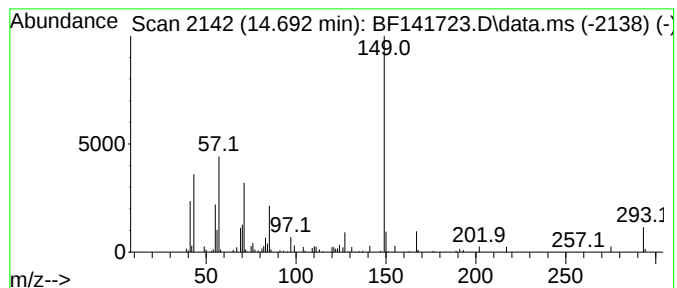
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Phthalic acid, nonyl 4-octyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.692	2.54 ng	63544	Perylene-d12	15.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, nonyl 4-octyl ester	404	C25H40O4	1000314-84-2	59
2			Phthalic acid, hept-3-yl nonyl e...	390	C24H38O4	1000356-99-3	53
3			Phthalic acid, 4,4-dimethylpent-...	390	C24H38O4	1000371-13-6	53
4			Phthalic acid, hept-4-yl nonyl e...	390	C24H38O4	1000356-79-0	53
5			Phthalic acid, butyl tetradecyl ...	418	C26H42O4	1000308-91-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022125\
Data File : BF141723.D
Acq On : 21 Feb 2025 16:47
Operator : RC/JU
Sample : Q1388-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12016

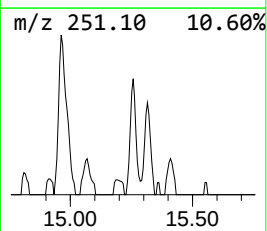
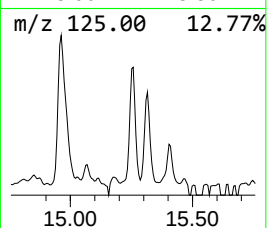
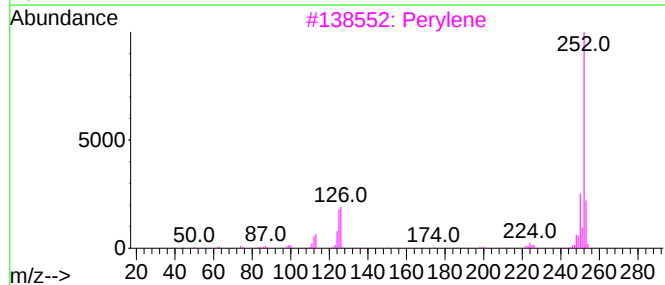
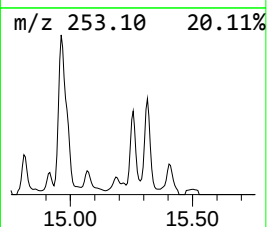
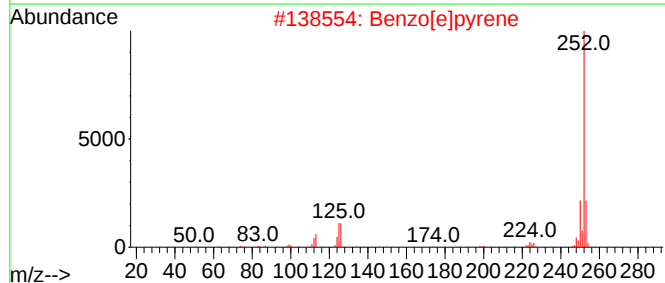
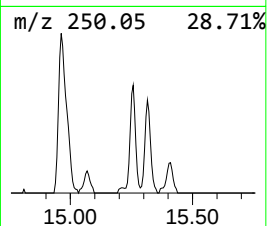
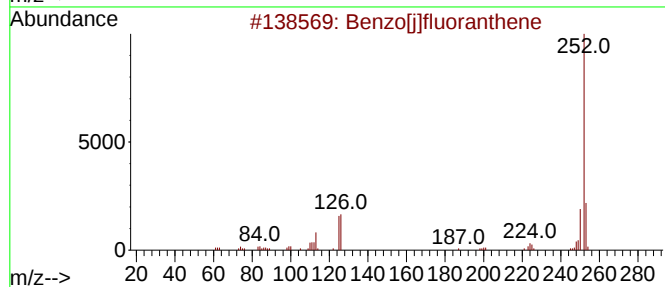
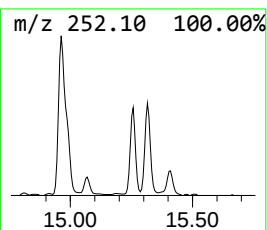
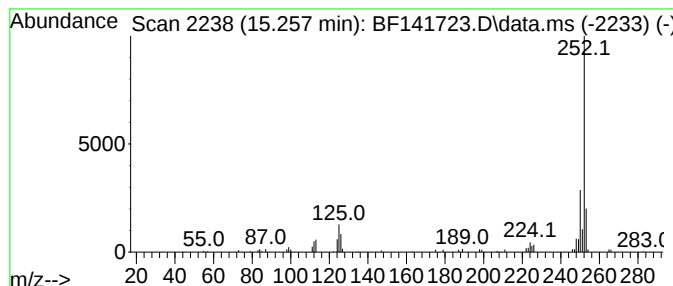
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[j]fluoranthene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.257	2.28 ng	57011	Perylene-d12	15.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
2			Benzo[e]pyrene	252	C20H12	000192-97-2	91
3			Perylene	252	C20H12	000198-55-0	90
4			Benzo[a]pyrene	252	C20H12	000050-32-8	90
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022125\
Data File : BF141723.D
Acq On : 21 Feb 2025 16:47
Operator : RC/JU
Sample : Q1388-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12016

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.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
Benzophenone	10.522	13.0	ng	530256	3	9.810	816815	20.0
n-Hexadecanoic ...	11.828	7.3	ng	351062	4	11.298	957515	20.0
Hexanedioic aci...	13.416	3.9	ng	134627	5	13.933	695797	20.0
1,3-Benzenedica...	14.557	3.3	ng	114415	5	13.933	695797	20.0
Phthalic acid, ...	14.692	2.5	ng	63544	6	15.374	500717	20.0
Benzo[j]fluoran...	15.257	2.3	ng	57011	6	15.374	500717	20.0