

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082322\
 Data File : BF129950.D
 Acq On : 23 Aug 2022 13:04
 Operator : CG\JU
 Sample : N4224-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP1-0816

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-BF081422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129950.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.004	459	462	476	rBV	174594	233593	8.12%	0.908%
2	5.416	528	532	556	rBV	2815331	2765784	96.12%	10.751%
3	6.434	701	705	720	rBV	2917114	2846231	98.92%	11.064%
4	6.775	759	763	773	rVB	1053627	854332	29.69%	3.321%
5	6.881	778	781	786	rVB	76699	66338	2.31%	0.258%
6	7.345	855	860	863	rBV	1973109	1781010	61.90%	6.923%
7	8.057	977	981	995	rVB	1305053	1159500	40.30%	4.507%
8	9.128	1158	1163	1167	rBV	3008649	2877377	100.00%	11.185%
9	9.810	1274	1279	1283	rBV	1585111	1315596	45.72%	5.114%
10	10.604	1410	1414	1428	rBV	2328979	2170014	75.42%	8.435%
11	11.298	1528	1532	1535	rBV	1453373	1300338	45.19%	5.055%
12	11.322	1535	1536	1541	rVB	65987	55679	1.94%	0.216%
13	11.363	1541	1543	1545	rBV	44028	35054	1.22%	0.136%
14	11.680	1593	1597	1599	rVB	63692	55264	1.92%	0.215%
15	11.822	1616	1621	1625	rBV2	52565	93674	3.26%	0.364%
16	12.516	1736	1739	1741	rBV	186335	168283	5.85%	0.654%
17	12.533	1741	1742	1745	rVB	66458	50869	1.77%	0.198%
18	12.692	1763	1769	1772	rVB	129904	115386	4.01%	0.449%
19	12.745	1772	1778	1781	rBV2	159288	186637	6.49%	0.725%
20	12.886	1797	1802	1805	rBV	3310446	2847807	98.97%	11.070%
21	13.098	1833	1838	1841	rVB2	43758	45774	1.59%	0.178%
22	13.398	1885	1889	1893	rBV	75699	76849	2.67%	0.299%
23	13.439	1893	1896	1898	rBV2	62085	53391	1.86%	0.208%
24	13.768	1947	1952	1954	rBV2	71788	76612	2.66%	0.298%
25	13.804	1954	1958	1971	rVB3	65813	152066	5.28%	0.591%
26	13.945	1978	1982	1986	rBV	1120874	1165893	40.52%	4.532%
27	13.974	1986	1987	1993	rVV	83951	57531	2.00%	0.224%
28	14.033	1993	1997	2000	rVV	49571	55212	1.92%	0.215%
29	14.080	2003	2005	2009	rVB	64412	57666	2.00%	0.224%
30	14.357	2046	2052	2053	rBV3	44258	70887	2.46%	0.276%
31	14.386	2053	2057	2059	rBV4	62490	78413	2.73%	0.305%
32	14.410	2059	2061	2062	rBV	41333	32261	1.12%	0.125%
33	14.427	2062	2064	2067	rVB	83712	65294	2.27%	0.254%
34	14.492	2069	2075	2077	rBV	293578	465202	16.17%	1.808%
35	14.574	2082	2089	2090	rVV	140417	249913	8.69%	0.971%
36	14.592	2090	2092	2095	rVV	174236	226553	7.87%	0.881%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082322\
Data File : BF129950.D
Acq On : 23 Aug 2022 13:04
Operator : CG\JU
Sample : N4224-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-0816

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-BF081422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.680	2099	2107	2112	rVV2	216629	529448	18.40%	2.058%
38	15.010	2156	2163	2169	rVB2	120864	276392	9.61%	1.074%
39	15.157	2184	2188	2192	rVB	58031	72114	2.51%	0.280%
40	15.286	2207	2210	2217	rVB	35629	45824	1.59%	0.178%
41	15.345	2217	2220	2223	rVV	51126	66991	2.33%	0.260%
42	15.404	2226	2230	2243	rVB	663360	826383	28.72%	3.212%

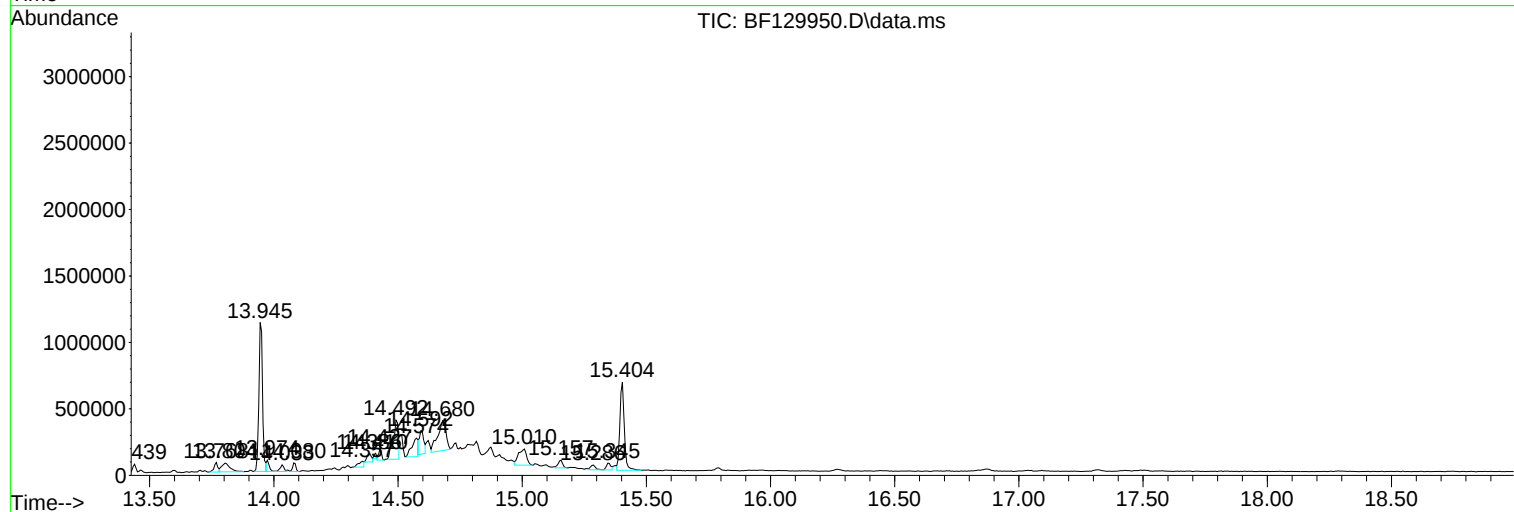
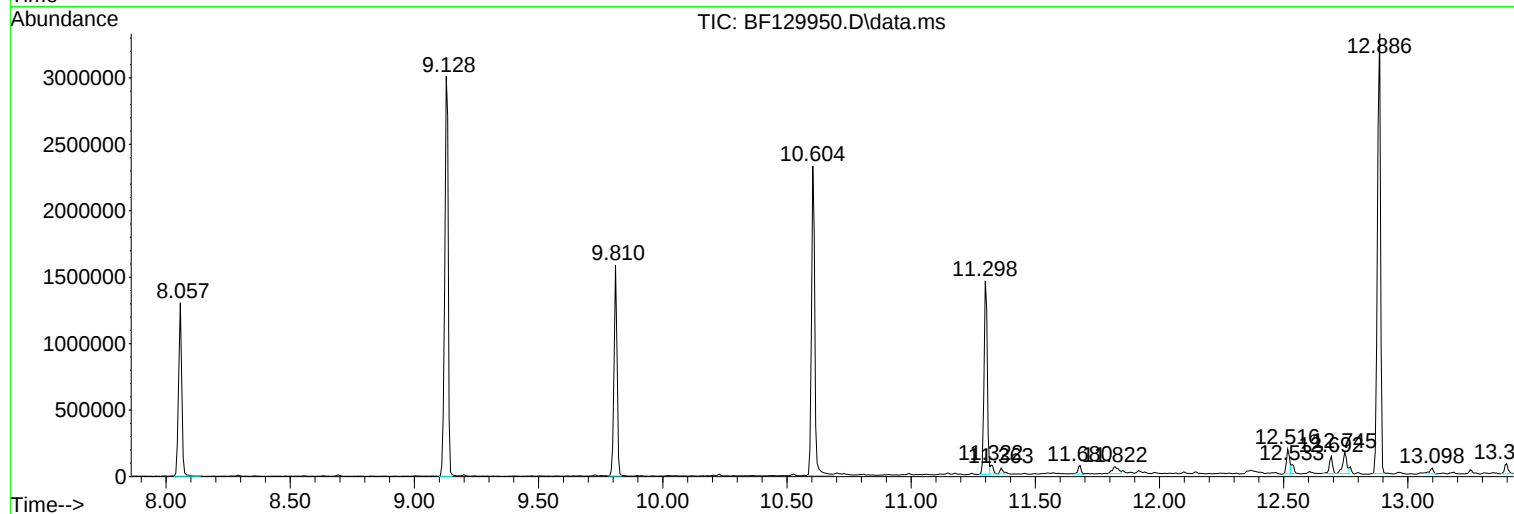
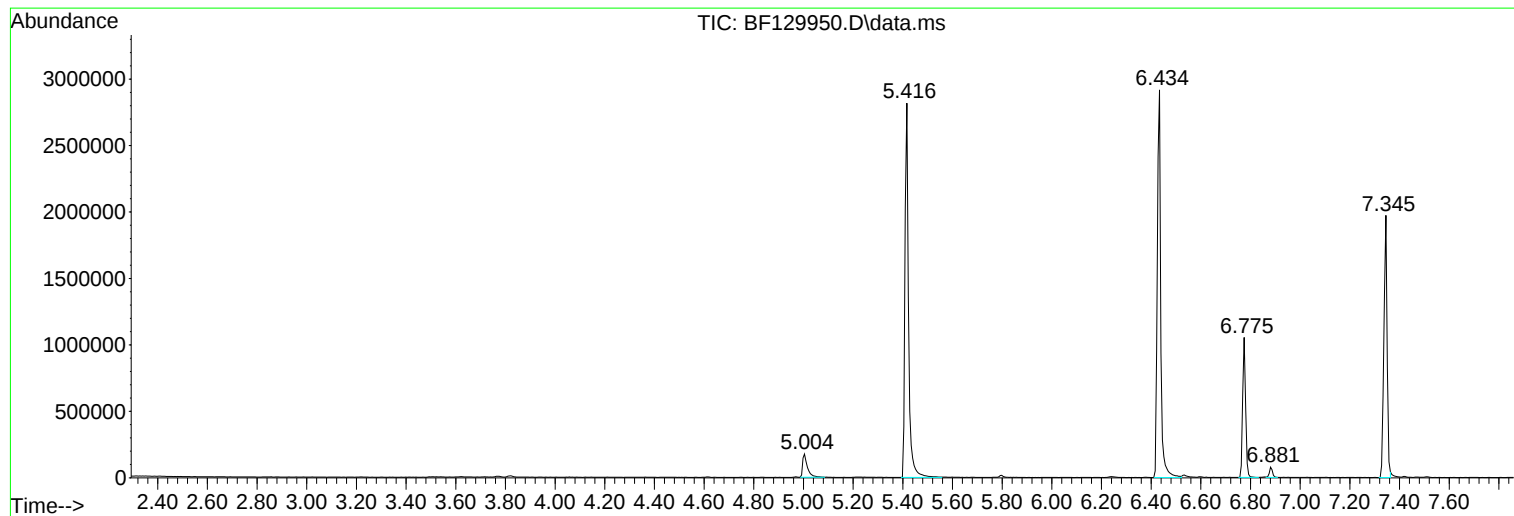
Sum of corrected areas: 25725435

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082322\
Data File : BF129950.D
Acq On : 23 Aug 2022 13:04
Operator : CG\JU
Sample : N4224-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-0816

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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\BF082322\
Data File : BF129950.D
Acq On : 23 Aug 2022 13:04
Operator : CG\JU
Sample : N4224-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-0816

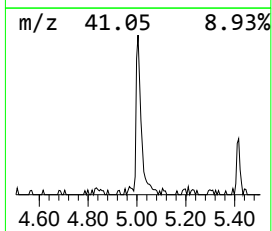
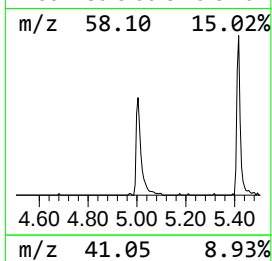
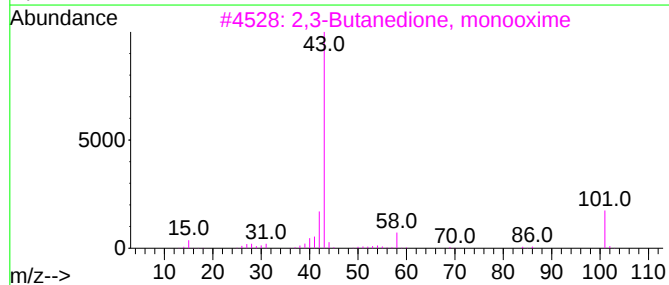
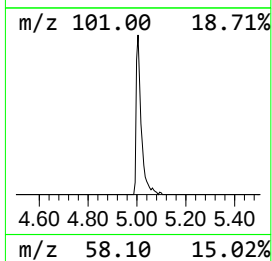
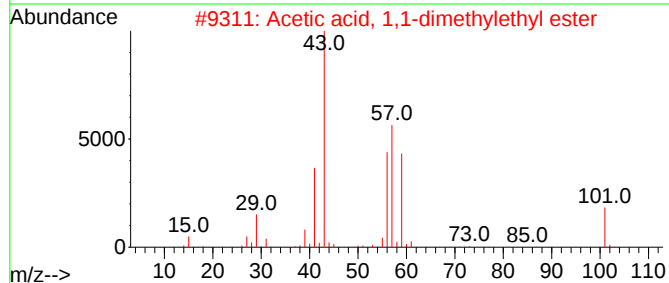
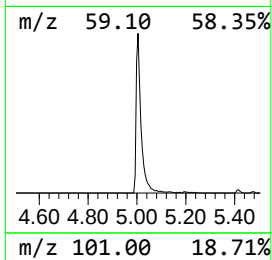
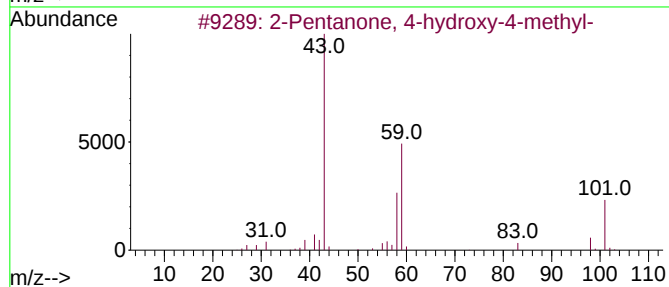
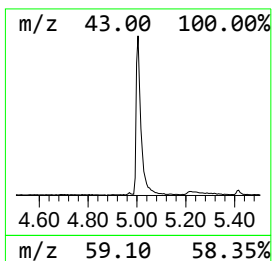
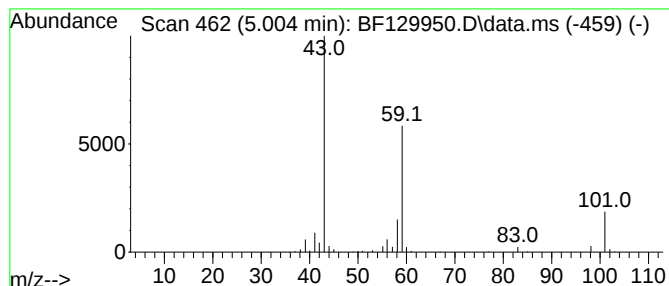
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.004	5.47 ng	233593	1,4-Dichlorobenzene-d4	6.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082322\
Data File : BF129950.D
Acq On : 23 Aug 2022 13:04
Operator : CG\JU
Sample : N4224-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-0816

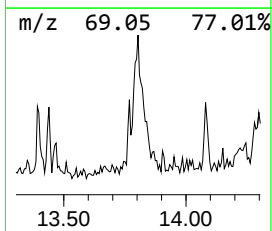
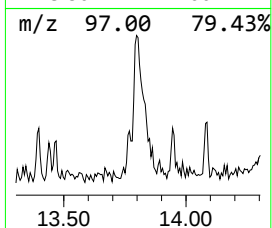
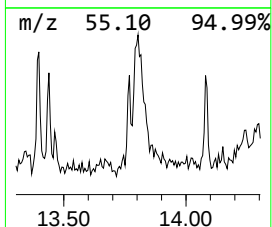
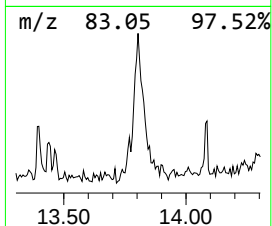
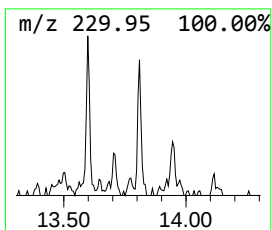
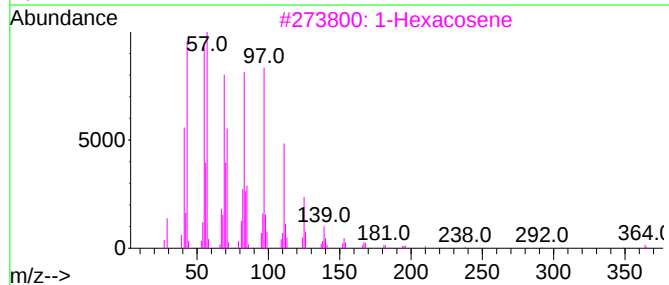
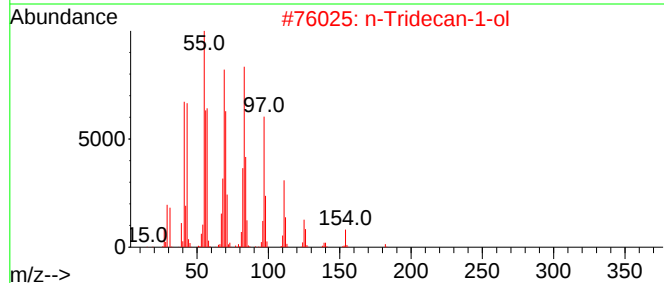
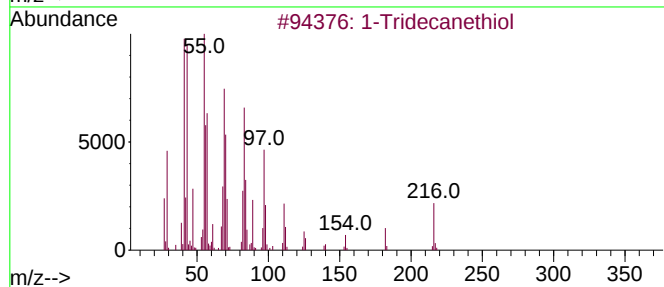
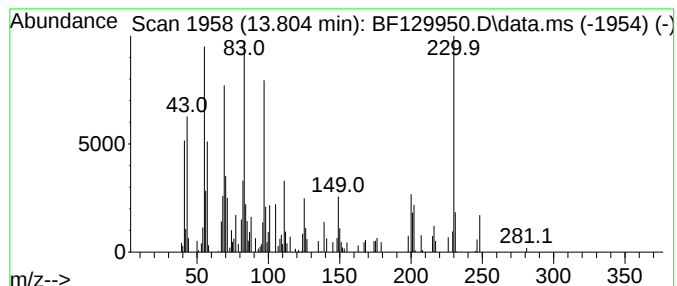
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown13.804 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.804	2.61 ng	152066	Chrysene-d12	13.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tridecanethiol	216	C13H28S	019484-26-5	49
2			n-Tridecan-1-ol	200	C13H28O	000112-70-9	49
3			1-Hexacosene	364	C26H52	018835-33-1	49
4			11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	46
5			Pentadec-7-ene, 7-bromomethyl-	302	C16H31Br	1000259-58-5	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082322\
Data File : BF129950.D
Acq On : 23 Aug 2022 13:04
Operator : CG\JU
Sample : N4224-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-0816

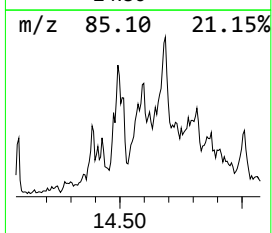
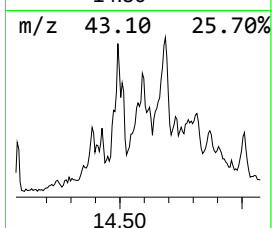
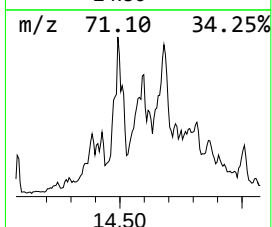
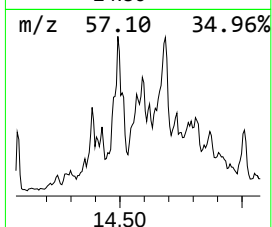
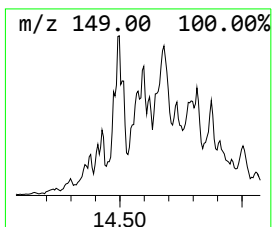
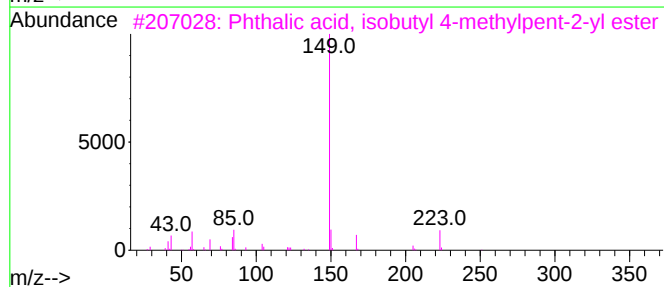
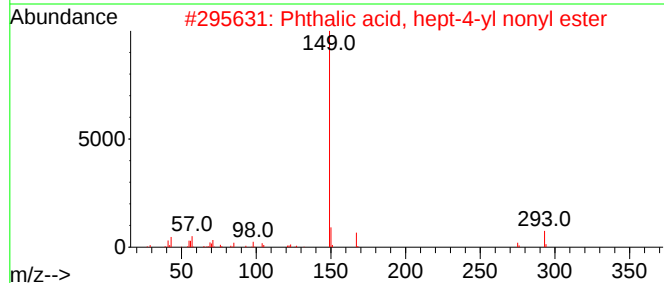
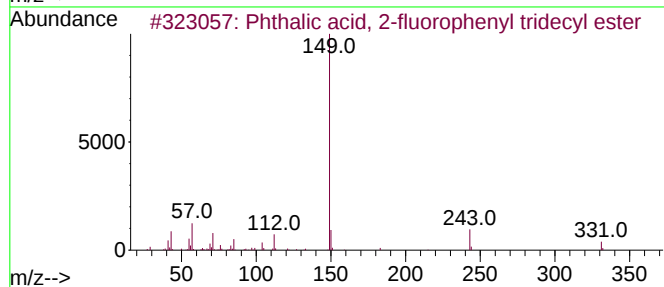
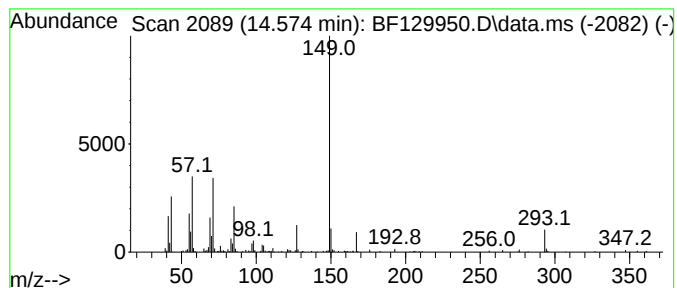
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Phthalic acid, 2-fluorophen... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.574	4.29 ng	249913	Chrysene-d12	13.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, 2-fluorophenyl tr...	442	C27H35F04	1000356-50-4	53
2			Phthalic acid, hept-4-yl nonyl e...	390	C24H3804	1000356-79-0	53
3			Phthalic acid, isobutyl 4-methyl...	306	C18H2604	1000356-87-2	53
4			Phthalic acid, 2,2-dimethylpent-...	404	C25H4004	1000415-53-3	50
5			Phthalic acid, 4-methylhept-3-yl...	390	C24H3804	1000377-94-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082322\
Data File : BF129950.D
Acq On : 23 Aug 2022 13:04
Operator : CG\JU
Sample : N4224-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-0816

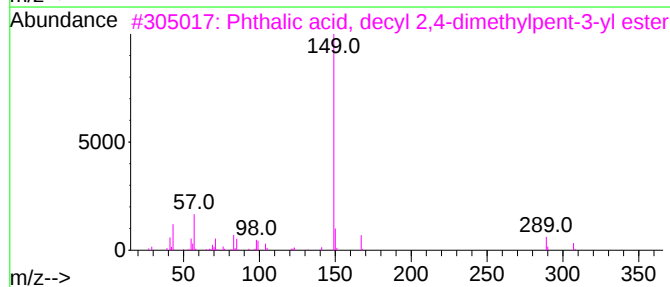
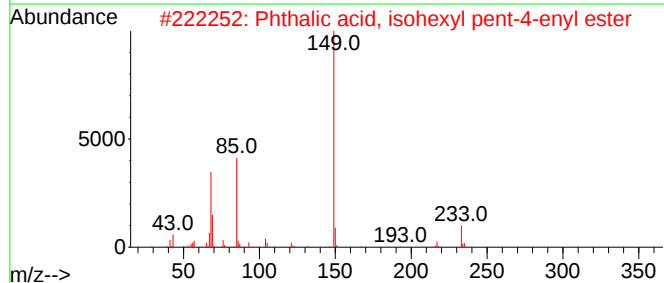
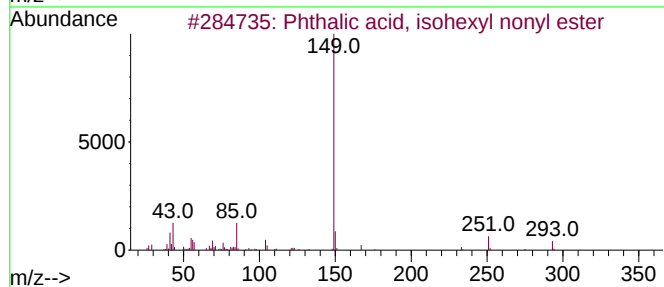
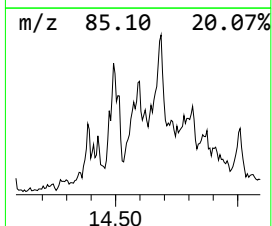
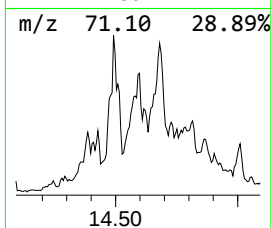
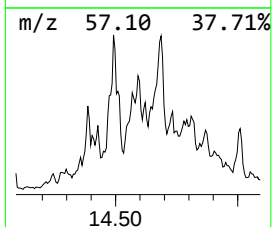
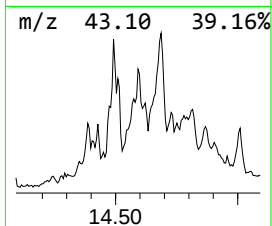
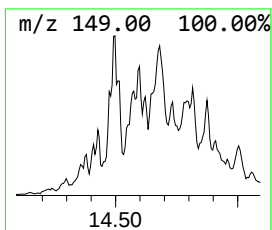
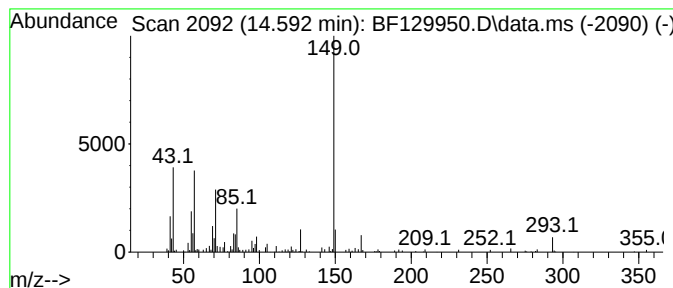
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Phthalic acid, isohexyl non... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.592	3.89 ng	226553	Chrysene-d12	13.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, isohexyl nonyl ester	376	C23H36O4	1000309-07-2	53
2			Phthalic acid, isohexyl pent-4-e...	318	C19H26O4	1000360-46-4	53
3			Phthalic acid, decyl 2,4-dimethy...	404	C25H40O4	1000356-84-9	50
4			Phthalic acid, dodecyl nonyl ester	460	C29H48O4	1000308-92-6	50
5			Phthalic acid, 4-methylpent-2-yl...	376	C23H36O4	1000356-87-9	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082322\
Data File : BF129950.D
Acq On : 23 Aug 2022 13:04
Operator : CG\JU
Sample : N4224-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

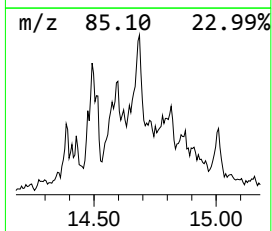
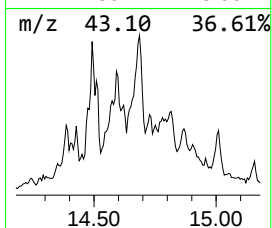
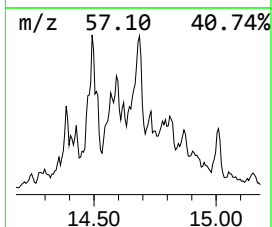
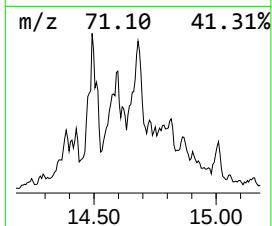
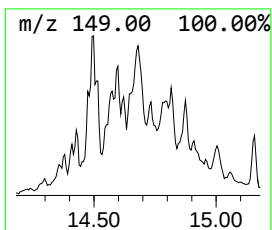
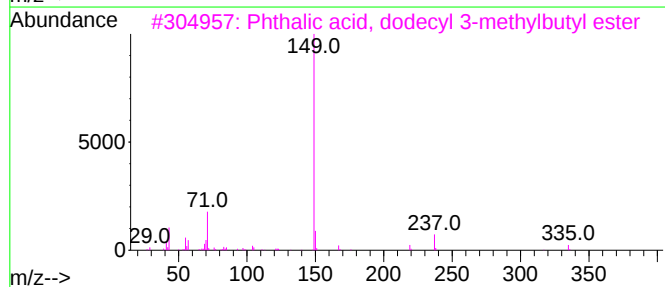
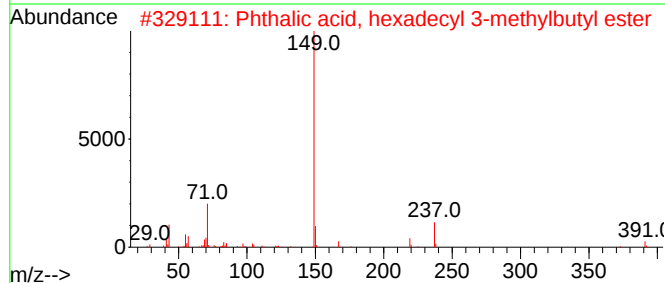
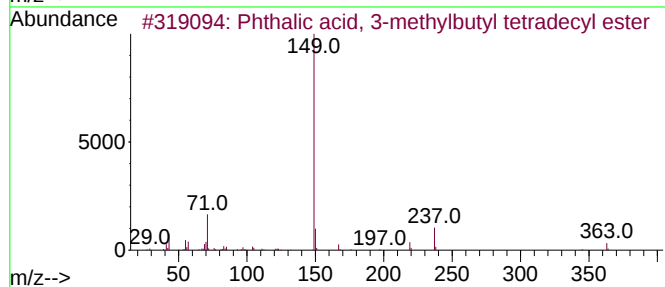
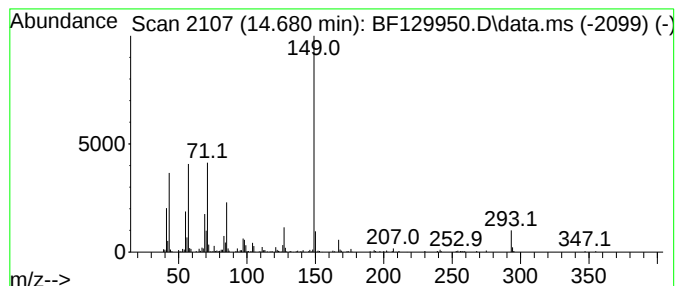
Instrument :
BNA_F
ClientSampleId :
TP1-0816

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Phthalic acid, 3-methylbuty... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.680	12.81 ng	529448	Perylene-d12	15.404	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, 3-methylbutyl tet...	432	C27H44O4	1000356-81-5	59
2	Phthalic acid, hexadecyl 3-methy...	460	C29H48O4	1000356-81-7	59
3	Phthalic acid, dodecyl 3-methylb...	404	C25H40O4	1000356-81-3	59
4	Phthalic acid, decyl 3-methylbut...	376	C23H36O4	1000356-81-1	53
5	Phthalic acid, cis-hex-3-enyl is...	332	C20H28O4	1000360-36-7	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082322\
Data File : BF129950.D
Acq On : 23 Aug 2022 13:04
Operator : CG\JU
Sample : N4224-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-0816

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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-...	5.004	5.5	ng	233593	1	6.775	854332	20.0
unknown13.804	13.804	2.6	ng	152066	5	13.951	1165890	20.0
Phthalic acid, ...	14.574	4.3	ng	249913	5	13.951	1165890	20.0
Phthalic acid, ...	14.592	3.9	ng	226553	5	13.951	1165890	20.0
Phthalic acid, ...	14.680	12.8	ng	529448	6	15.404	826383	20.0