

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
 Data File : BF125952.D
 Acq On : 27 Oct 2021 00:55
 Operator : JU/CG
 Sample : M4316-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-2-IS

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-BF102521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125952.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	6	13	19	rBV	1955065	2498364	60.19%	8.076%
2	3.357	213	216	227	rBV2	22411	48618	1.17%	0.157%
3	3.946	307	316	321	rBV4	28605	63366	1.53%	0.205%
4	5.087	507	510	515	rVB	40095	50369	1.21%	0.163%
5	5.481	569	577	580	rBV	4338004	4150803	100.00%	13.418%
6	6.398	730	733	736	rBV	61617	68869	1.66%	0.223%
7	6.428	736	738	741	rVB2	58951	46920	1.13%	0.152%
8	6.487	742	748	751	rBV	3978604	4099557	98.77%	13.252%
9	6.557	756	760	767	rVB	67560	60671	1.46%	0.196%
10	6.692	780	783	788	rBV	267773	216276	5.21%	0.699%
11	6.863	809	812	815	rBV	1175692	1039762	25.05%	3.361%
12	6.928	820	823	826	rBV	94152	80142	1.93%	0.259%
13	7.187	863	867	870	rBV3	69687	63002	1.52%	0.204%
14	7.428	898	908	911	rBV	2745077	2665282	64.21%	8.616%
15	7.510	917	922	927	rVB5	28567	42024	1.01%	0.136%
16	7.639	939	944	946	rBV3	41647	47019	1.13%	0.152%
17	8.051	1010	1014	1017	rBV	1092229	764494	18.42%	2.471%
18	8.145	1026	1030	1033	rBV	1457425	1347700	32.47%	4.357%
19	8.857	1145	1151	1154	rVB	61941	55131	1.33%	0.178%
20	9.222	1209	1213	1217	rBV	3586128	3226382	77.73%	10.430%
21	9.898	1325	1328	1332	rVB	1426057	1298135	31.27%	4.196%
22	10.192	1374	1378	1386	rVB	83913	99474	2.40%	0.322%
23	10.686	1458	1462	1465	rBV	2390827	2031425	48.94%	6.567%
24	11.386	1577	1581	1584	rBV	1320521	1114216	26.84%	3.602%
25	11.786	1646	1649	1653	rBV	64250	50578	1.22%	0.163%
26	11.910	1667	1670	1677	rBV	142970	148740	3.58%	0.481%
27	12.492	1763	1769	1772	rBV2	109496	128803	3.10%	0.416%
28	12.698	1801	1804	1807	rBV2	71677	65858	1.59%	0.213%
29	12.974	1847	1851	1854	rBV	2463811	2301922	55.46%	7.441%
30	13.216	1889	1892	1895	rBV2	79492	70087	1.69%	0.227%
31	13.874	2001	2004	2011	rBV2	280085	315976	7.61%	1.021%
32	14.021	2025	2029	2032	rBV	1097235	965636	23.26%	3.121%
33	14.204	2057	2060	2063	rVB2	53998	61961	1.49%	0.200%
34	14.510	2109	2112	2119	rBV	259275	294363	7.09%	0.952%
35	14.821	2162	2165	2166	rBV2	50044	48567	1.17%	0.157%
36	15.492	2274	2279	2283	rBV	768392	896701	21.60%	2.899%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125952.D
Acq On : 27 Oct 2021 00:55
Operator : JU/CG
Sample : M4316-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2-IS

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-BF102521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.992	2361	2364	2367	rBV	58780	64166	1.55%	0.207%
38	16.039	2368	2372	2377	rVB4	76389	116570	2.81%	0.377%
39	16.221	2400	2403	2411	rVB3	88056	140706	3.39%	0.455%
40	16.668	2475	2479	2484	rVB8	53456	86492	2.08%	0.280%

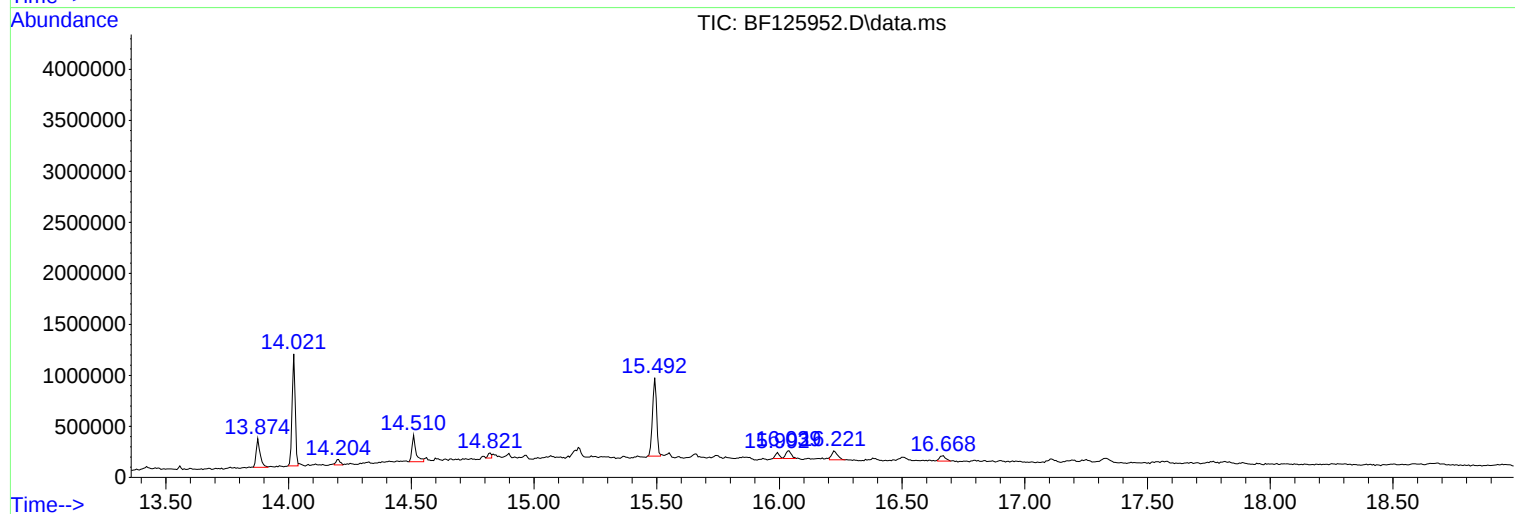
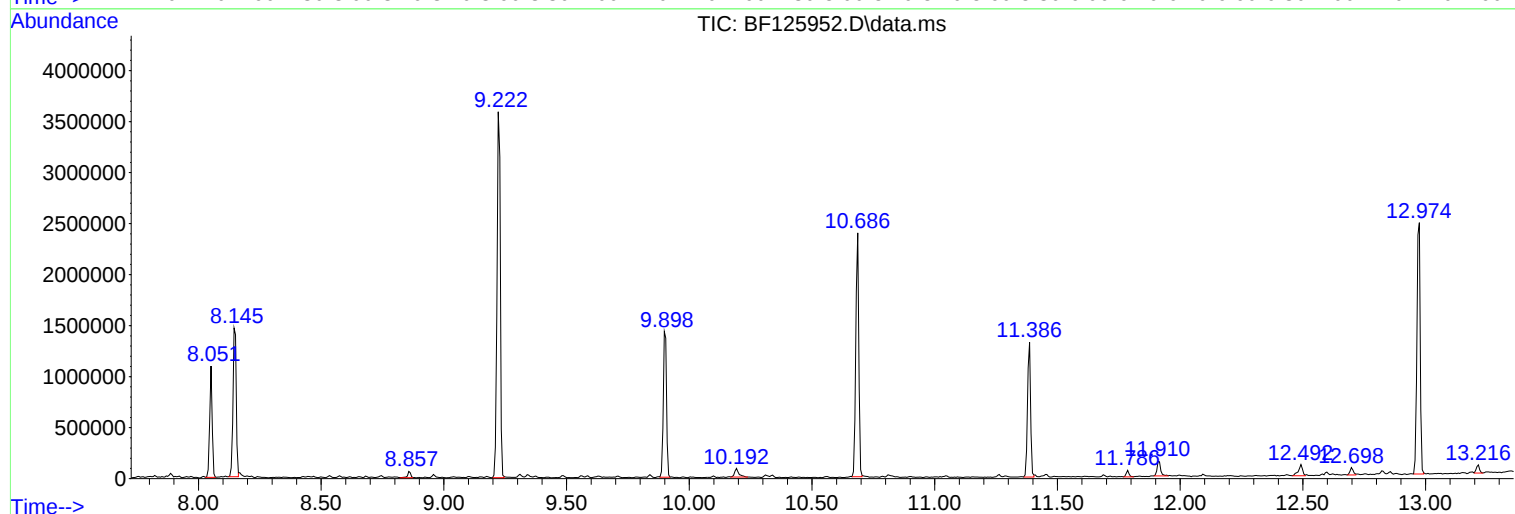
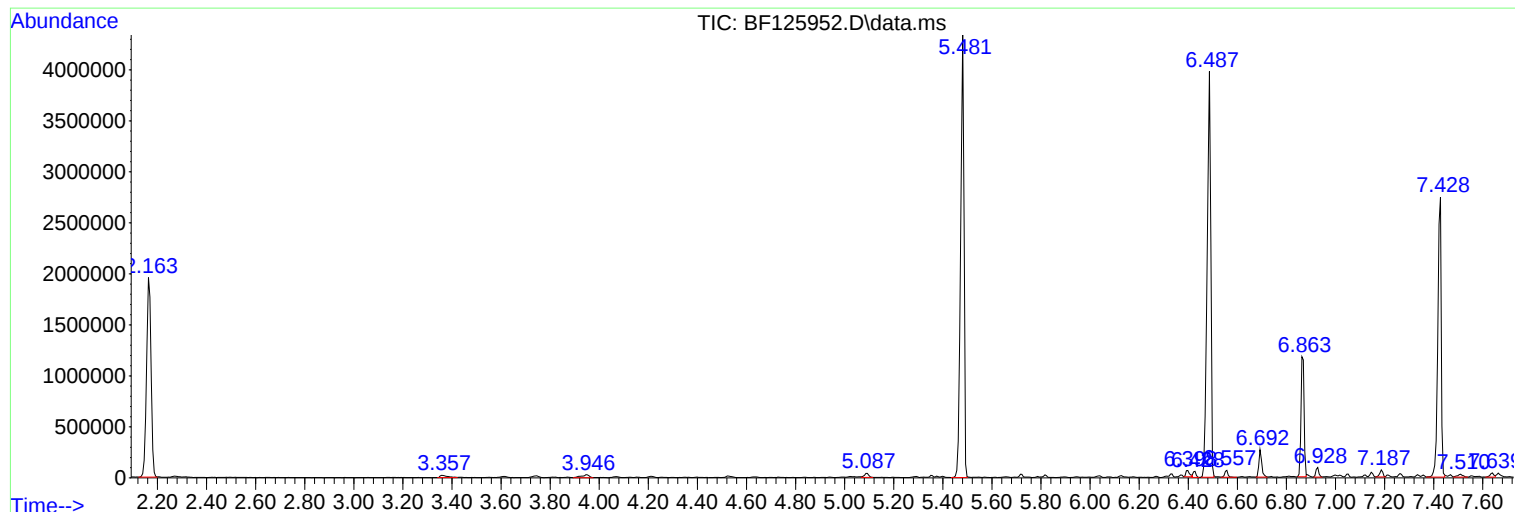
Sum of corrected areas: 30935127

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125952.D
Acq On : 27 Oct 2021 00:55
Operator : JU/CG
Sample : M4316-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2-IS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.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\BF102621\
Data File : BF125952.D
Acq On : 27 Oct 2021 00:55
Operator : JU/CG
Sample : M4316-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2-IS

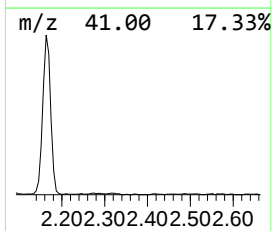
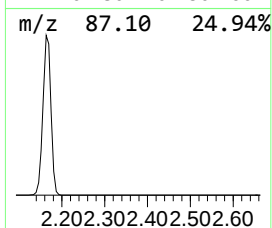
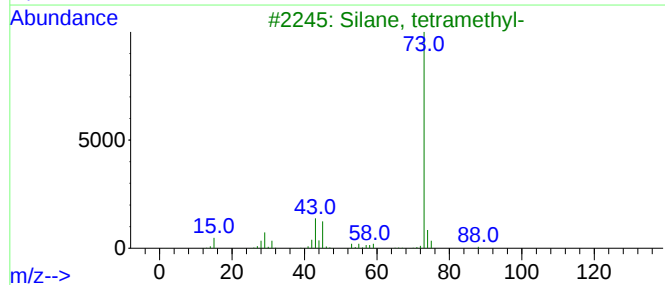
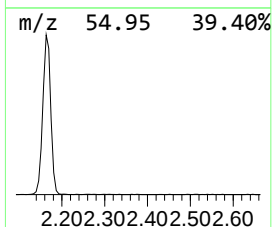
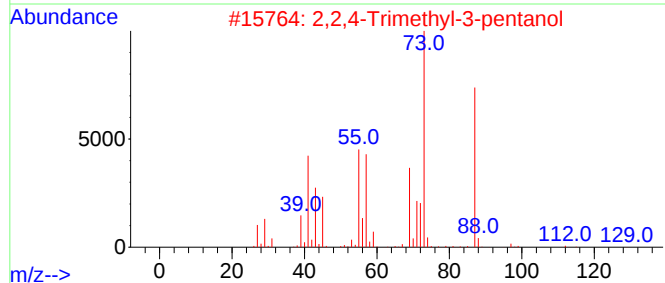
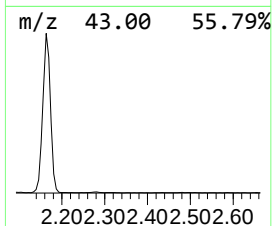
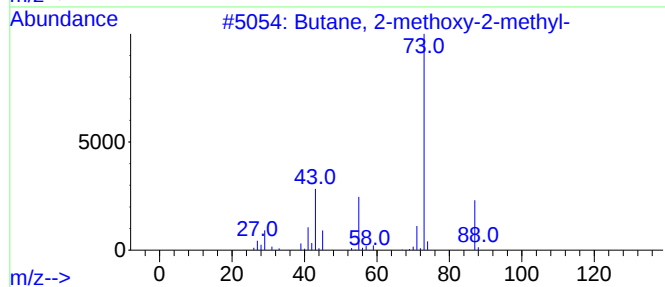
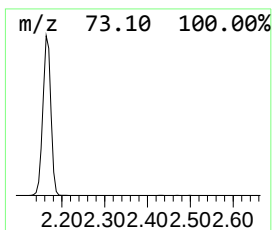
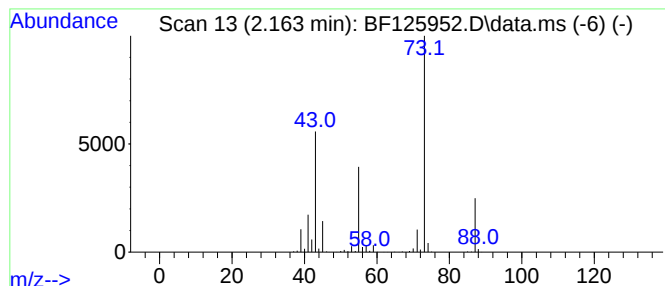
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	48.06 ng	2498360	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125952.D
Acq On : 27 Oct 2021 00:55
Operator : JU/CG
Sample : M4316-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2-IS

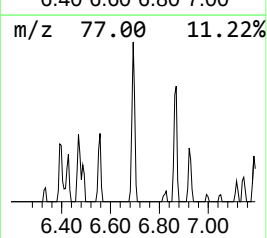
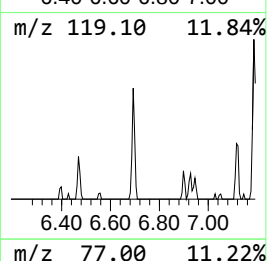
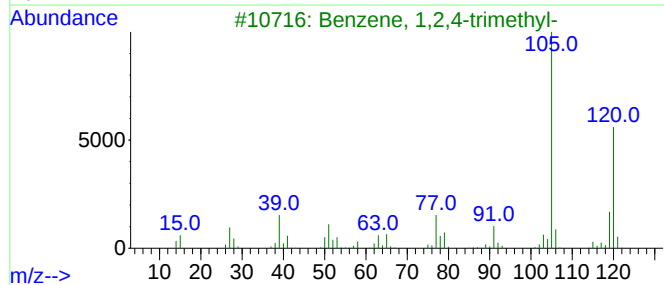
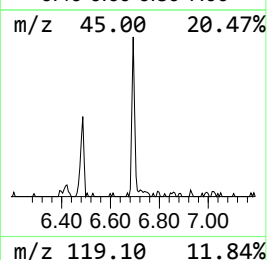
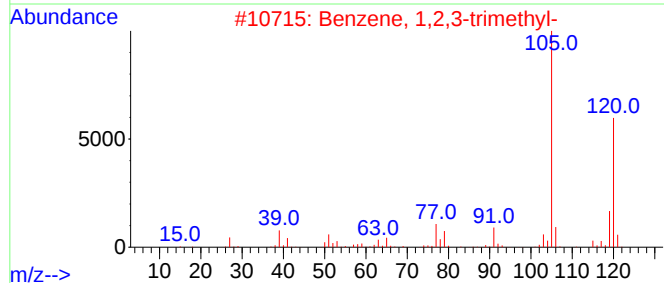
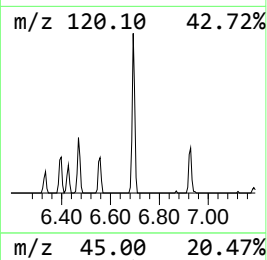
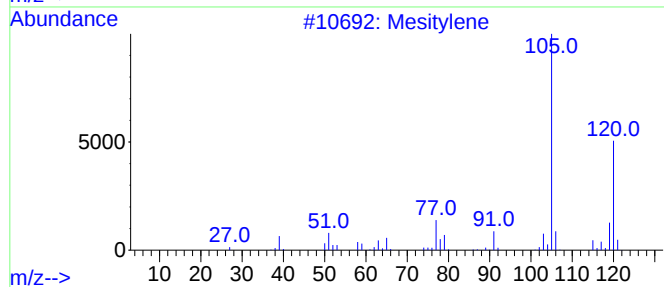
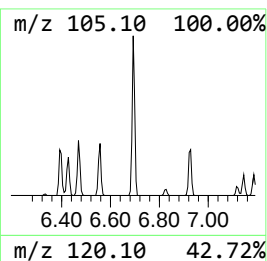
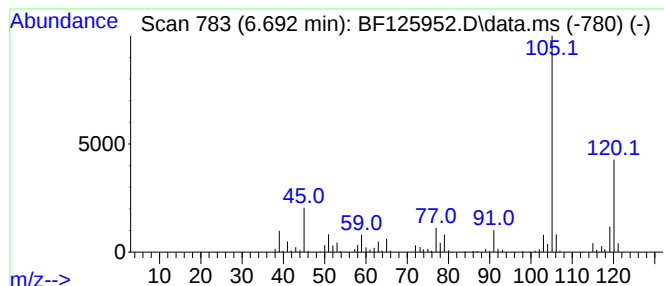
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Mesitylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.692	4.16 ng	216276	1,4-Dichlorobenzene-d4	6.869

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Mesitylene	120	C9H12	000108-67-8	95
2		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
5		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125952.D
Acq On : 27 Oct 2021 00:55
Operator : JU/CG
Sample : M4316-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2-IS

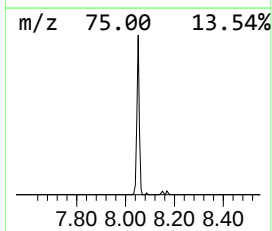
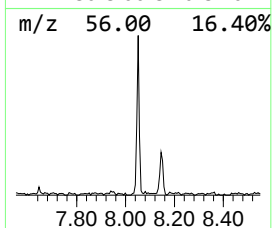
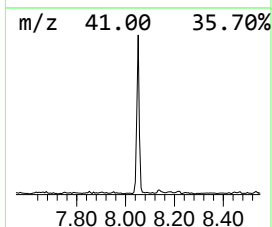
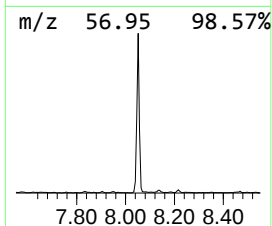
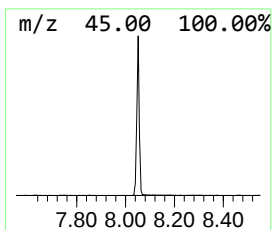
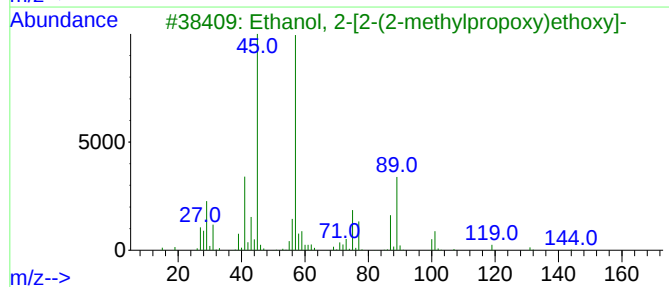
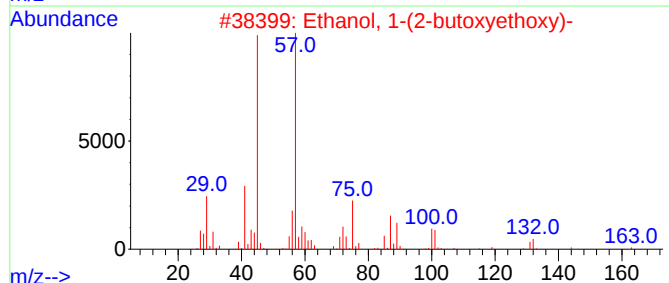
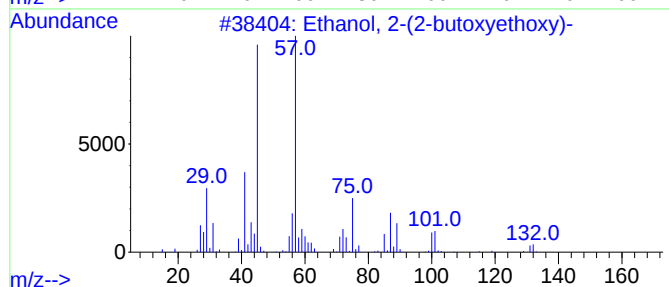
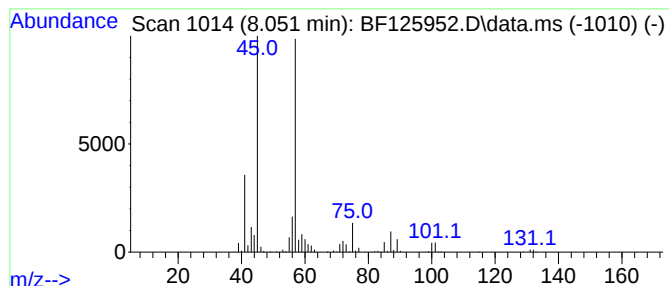
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	11.35 ng	764494	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
4			Pentaethylene glycol	238	C10H22O6	004792-15-8	50
5			2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125952.D
Acq On : 27 Oct 2021 00:55
Operator : JU/CG
Sample : M4316-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2-IS

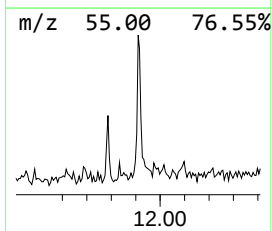
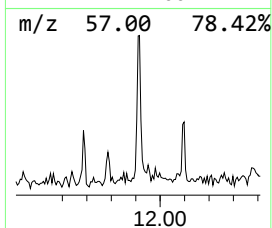
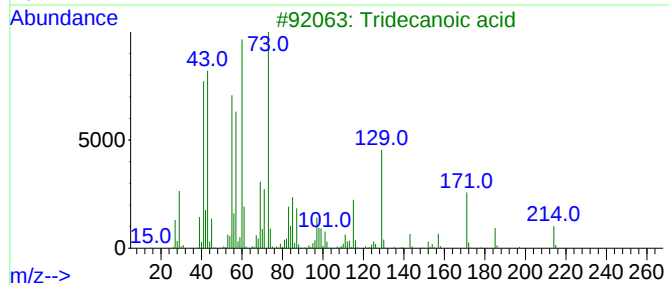
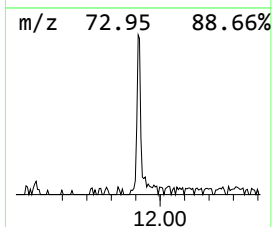
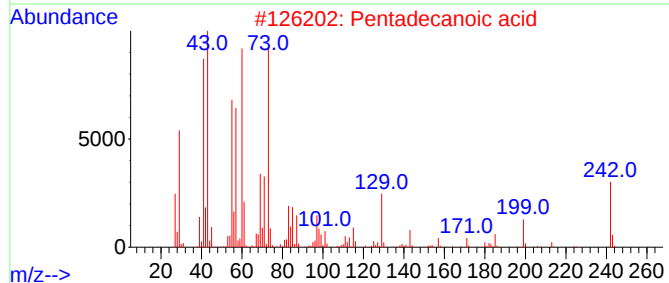
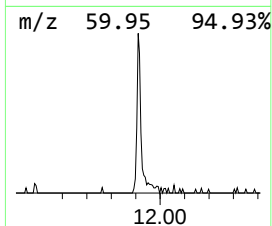
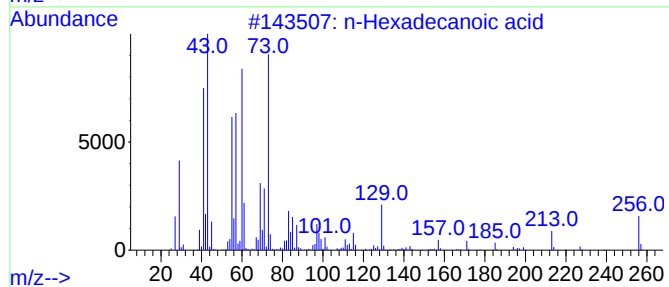
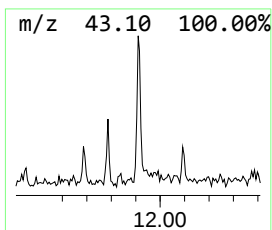
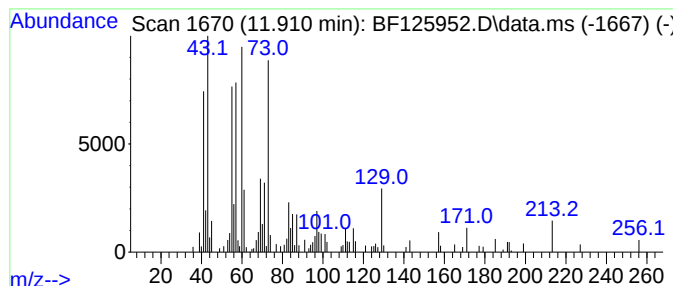
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	2.67 ng	148740	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3			Tridecanoic acid	214	C13H26O2	000638-53-9	59
4			Undecanoic acid	186	C11H22O2	000112-37-8	58
5			Dodecanoic acid	200	C12H24O2	000143-07-7	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125952.D
Acq On : 27 Oct 2021 00:55
Operator : JU/CG
Sample : M4316-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2-IS

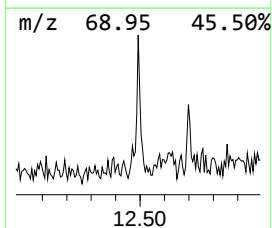
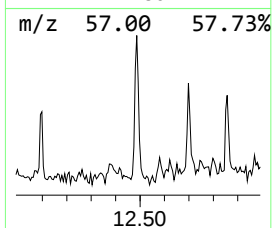
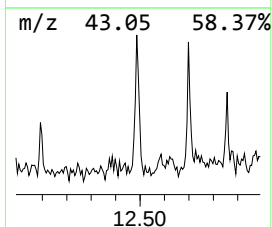
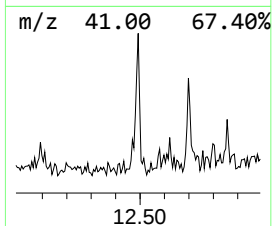
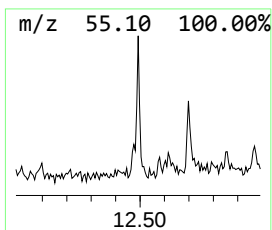
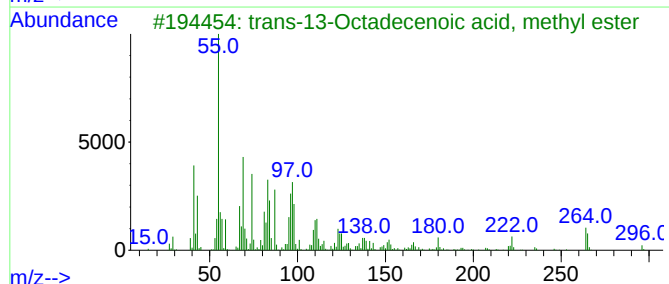
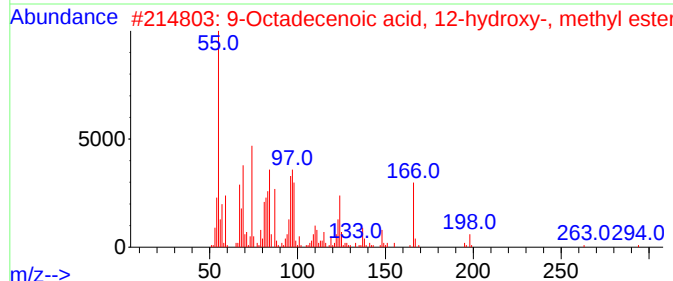
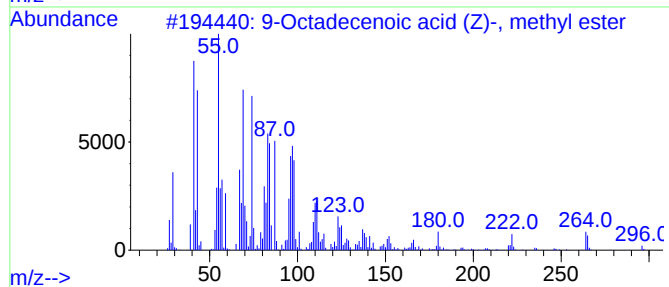
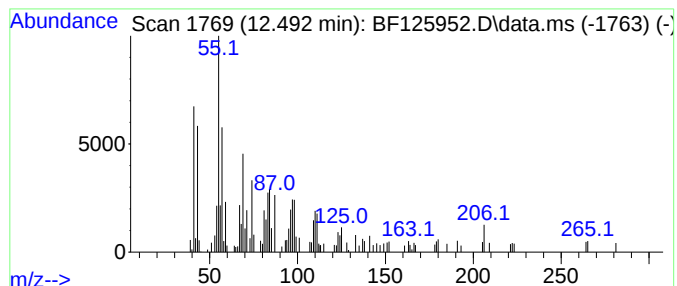
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.492	2.31 ng	128803	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	76
2			9-Octadecenoic acid, 12-hydroxy-...	312	C19H36O3	000141-24-2	52
3			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	52
4			11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	49
5			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125952.D
Acq On : 27 Oct 2021 00:55
Operator : JU/CG
Sample : M4316-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2-IS

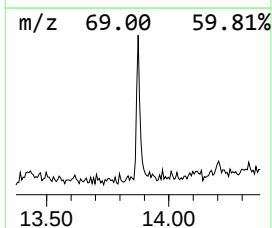
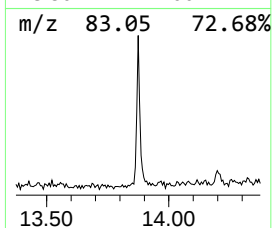
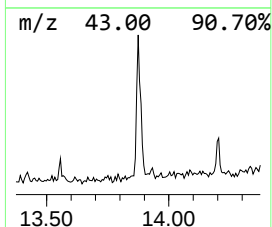
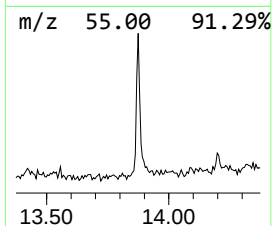
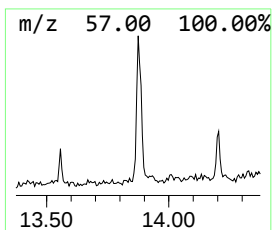
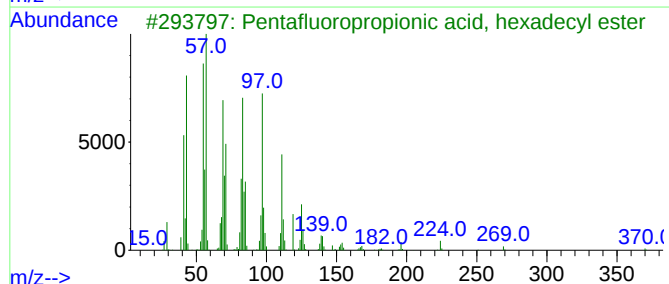
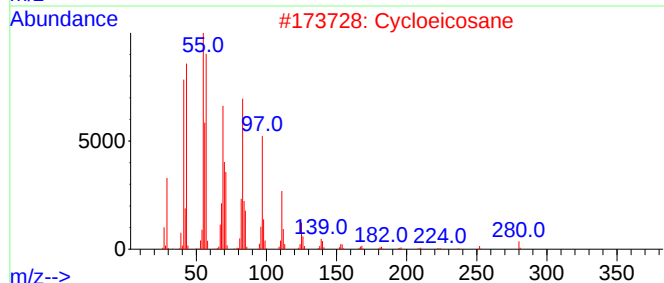
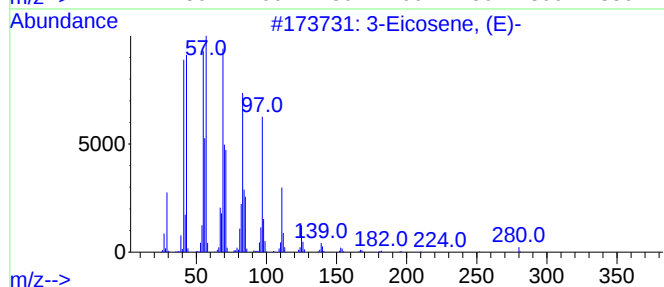
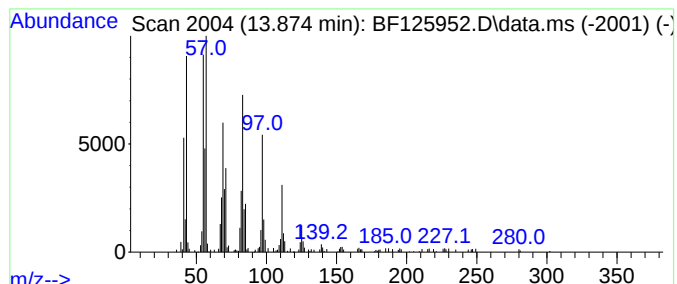
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 3-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	6.54 ng	315976	Chrysene-d12	14.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Eicosene, (E)-	280	C20H40	074685-33-9	94
2			Cycloeicosane	280	C20H40	000296-56-0	94
3			Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	91
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5			1-Heneicosanol	312	C21H44O	015594-90-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125952.D
Acq On : 27 Oct 2021 00:55
Operator : JU/CG
Sample : M4316-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2-IS

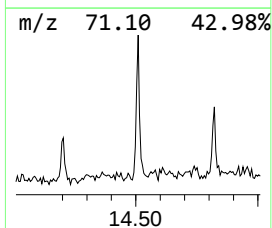
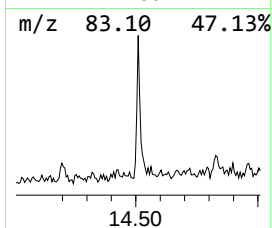
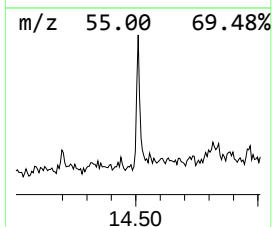
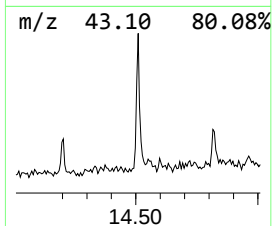
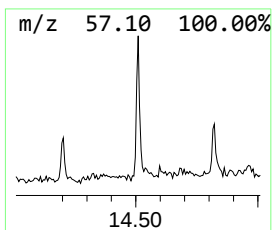
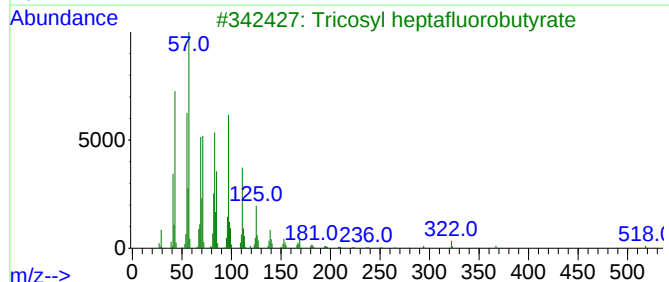
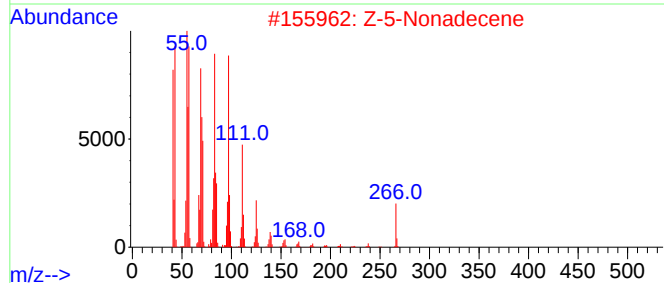
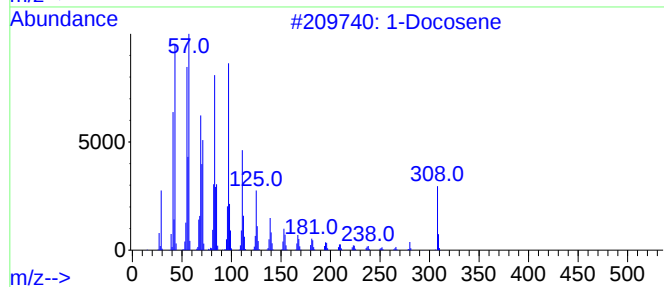
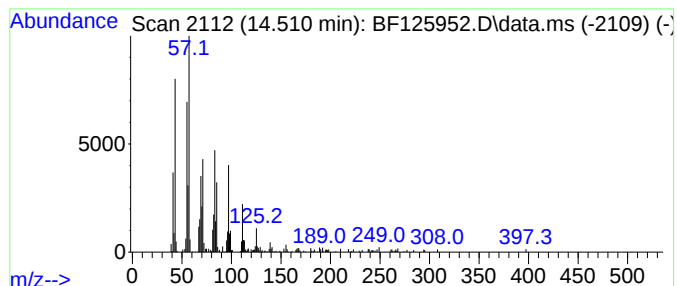
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.510	6.10 ng	294363	Chrysene-d12	14.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	95
2	Z-5-Nonadecene			266	C19H38	1000131-11-8	95
3	Tricosyl heptafluorobutyrate			536	C27H47F7O2	1000351-83-4	91
4	Triacontyl trifluoroacetate			534	C32H61F3O2	1000351-75-7	91
5	Docosyl pentafluoropropionate			472	C25H45F5O2	1000351-80-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125952.D
Acq On : 27 Oct 2021 00:55
Operator : JU/CG
Sample : M4316-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

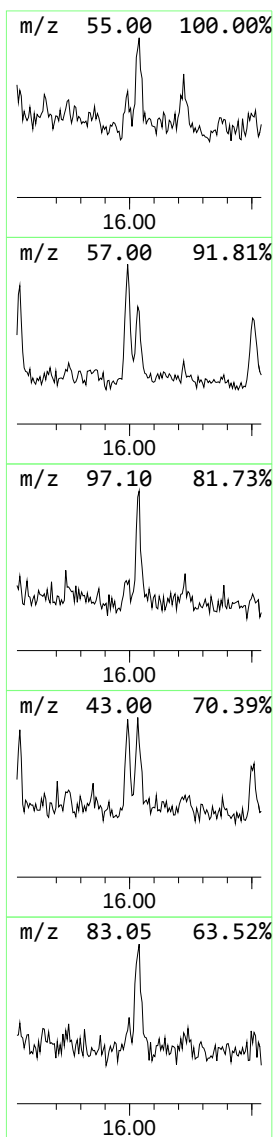
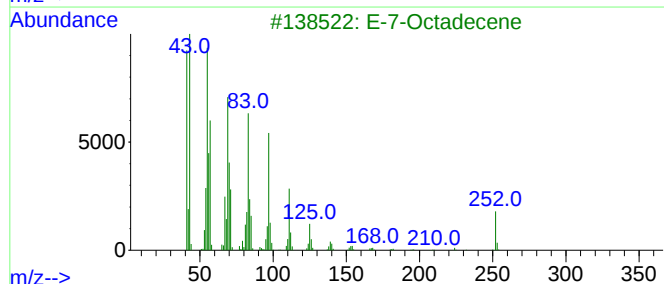
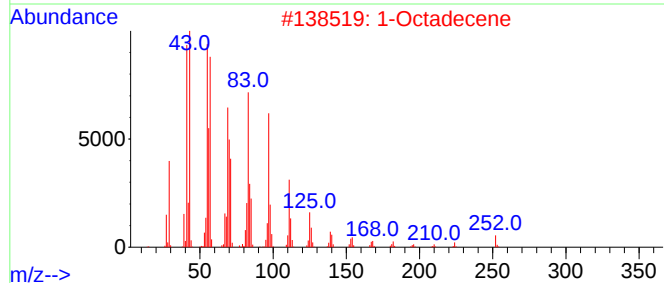
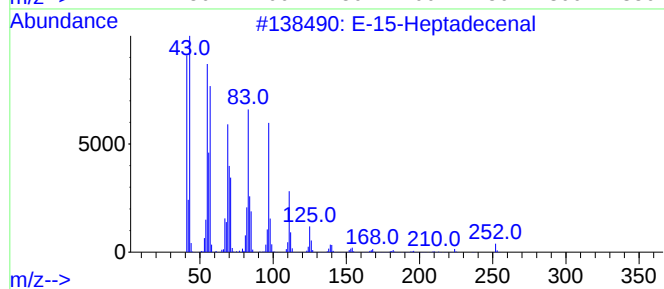
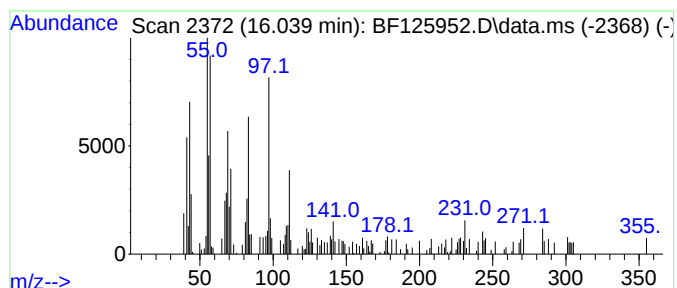
Instrument :
BNA_F
ClientSampleId :
WC-2-IS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 E-15-Heptadecenal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.039	2.60 ng	116570	Perylene-d12		15.492	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal		252	C17H32O	1000130-97-9	87
2	1-Octadecene		252	C18H36	000112-88-9	68
3	E-7-Octadecene		252	C18H36	1000130-92-0	58
4	n-Tetracosanol-1		354	C24H50O	000506-51-4	49
5	Cyclohexane, 1,1,2-trimethyl-		126	C9H18	007094-26-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125952.D
Acq On : 27 Oct 2021 00:55
Operator : JU/CG
Sample : M4316-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

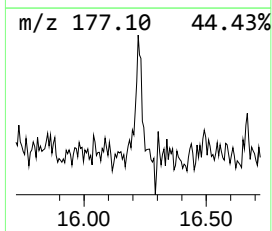
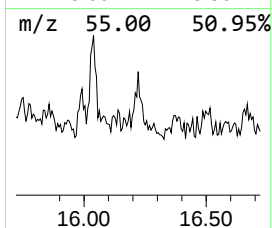
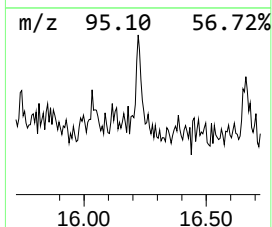
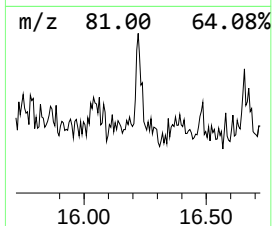
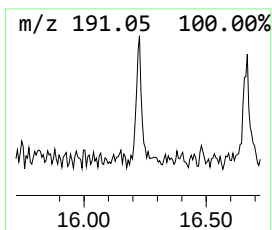
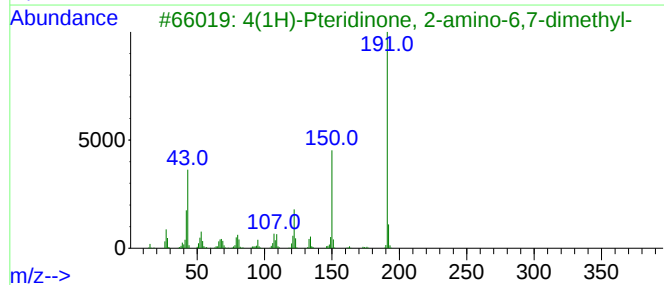
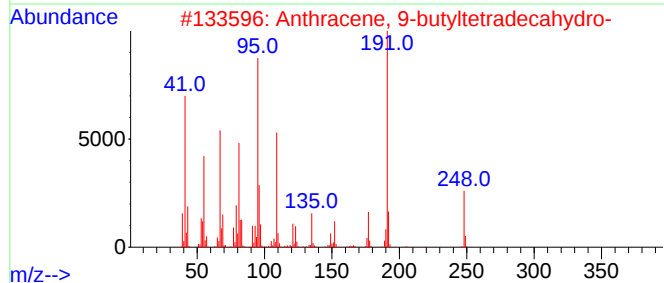
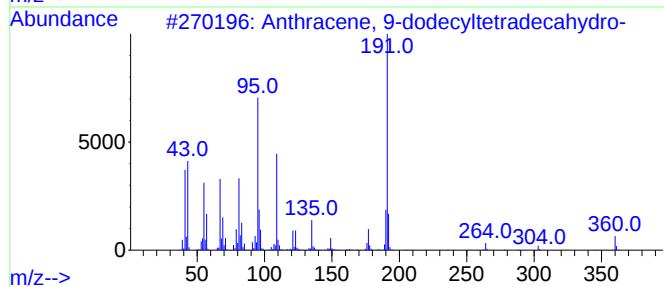
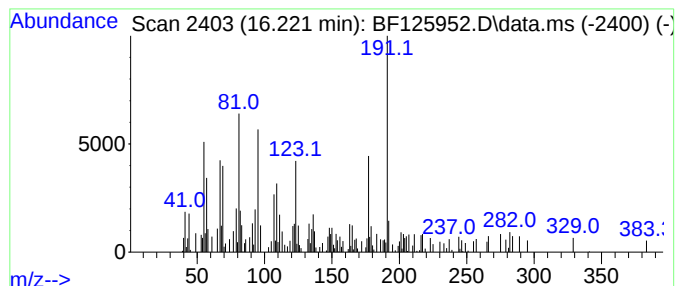
Instrument :
BNA_F
ClientSampleId :
WC-2-IS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown16.221 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.221	3.14 ng	140706	Perylene-d12	15.492
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		Anthracene, 9-dodecyltetradecahy...	360 C26H48	055401-75-7 47
2		Anthracene, 9-butyltetradecahydro-	248 C18H32	055133-89-6 38
3		4(1H)-Pteridinone, 2-amino-6,7-d...	191 C8H9N5O	000611-55-2 25
4		N-[[2-Oxo-1,2'-bi(tricyclo[3.3.1...	355 C23H33NO2	1000305-39-6 22
5		2-Amino-4-methyl-6-(2-thienyl)py...	191 C9H9N3S	026963-43-9 18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125952.D
Acq On : 27 Oct 2021 00:55
Operator : JU/CG
Sample : M4316-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2-IS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.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
Butane, 2-metho...	2.163	48.1	ng	2498360	1	6.869	1039760	20.0
Mesitylene	6.692	4.2	ng	216276	1	6.869	1039760	20.0
Ethanol, 2-(2-b...	8.051	11.4	ng	764494	2	8.151	1347700	20.0
n-Hexadecanoic ...	11.910	2.7	ng	148740	4	11.386	1114220	20.0
9-Octadecenoic ...	12.492	2.3	ng	128803	4	11.386	1114220	20.0
3-Eicosene, (E)-	13.874	6.5	ng	315976	5	14.021	965636	20.0
1-Docosene	14.510	6.1	ng	294363	5	14.021	965636	20.0
E-15-Heptadecenal	16.039	2.6	ng	116570	6	15.492	896701	20.0
unknown16.221	16.221	3.1	ng	140706	6	15.492	896701	20.0