

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
 Data File : BF122425.D
 Acq On : 21 Nov 2020 17:36
 Operator : JU/CG
 Sample : L4829-09
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-9

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-BF110920.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122425.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	4	10	18	rVB	1493362	1910995	25.60%	3.530%
2	4.593	421	426	429	rBV	82593	85272	1.14%	0.158%
3	5.481	573	577	581	rBV	3076448	2854029	38.23%	5.272%
4	6.034	668	671	675	rVB	156944	123367	1.65%	0.228%
5	6.493	744	749	755	rBV2	2160621	2287950	30.64%	4.226%
6	6.551	755	759	762	rVB	522732	446225	5.98%	0.824%
7	6.863	808	812	815	rBV	1449699	1163078	15.58%	2.148%
8	7.122	852	856	861	rVB2	114817	122881	1.65%	0.227%
9	7.428	899	908	914	rBV2	4218929	4823168	64.60%	8.909%
10	7.822	972	975	980	rVB	160671	153877	2.06%	0.284%
11	7.887	982	986	991	rVV2	186672	187573	2.51%	0.346%
12	8.151	1017	1031	1033	rBV	1682500	1825854	24.45%	3.373%
13	8.169	1033	1034	1036	rVV2	263170	179698	2.41%	0.332%
14	8.198	1036	1039	1041	rVV	191418	189357	2.54%	0.350%
15	8.222	1041	1043	1048	rVB	135627	120166	1.61%	0.222%
16	8.534	1093	1096	1101	rVB	104853	84046	1.13%	0.155%
17	8.957	1164	1168	1172	rBV3	192336	183215	2.45%	0.338%
18	9.228	1209	1214	1217	rBV	6919511	7063445	94.60%	13.048%
19	9.622	1277	1281	1284	rBV	266916	253756	3.40%	0.469%
20	9.904	1322	1329	1333	rBV	1881301	1807140	24.20%	3.338%
21	10.698	1459	1464	1467	rBV	4756659	4487772	60.11%	8.290%
22	11.392	1578	1582	1586	rBV	2135776	1902804	25.49%	3.515%
23	11.933	1666	1674	1698	rBV	2028109	3091847	41.41%	5.711%
24	12.586	1781	1785	1788	rBV	75958	88790	1.19%	0.164%
25	12.639	1789	1794	1800	rBV7	57403	157444	2.11%	0.291%
26	12.722	1802	1808	1820	rBV	3195326	4768191	63.86%	8.808%
27	12.992	1848	1854	1857	rBV	7333510	7466256	100.00%	13.792%
28	13.222	1889	1893	1896	rBV	68420	75729	1.01%	0.140%
29	13.563	1945	1951	1954	rBV2	92021	95531	1.28%	0.176%
30	13.892	2003	2007	2026	rBV	820754	1325800	17.76%	2.449%
31	14.039	2028	2032	2039	rVB	2314930	2055515	27.53%	3.797%
32	14.210	2058	2061	2070	rBV	116733	129827	1.74%	0.240%
33	14.516	2108	2113	2115	rBV2	125006	131807	1.77%	0.243%
34	14.827	2163	2166	2170	rVB	115164	105540	1.41%	0.195%
35	15.174	2221	2225	2232	rVB	125564	171929	2.30%	0.318%
36	15.516	2278	2283	2288	rBV	1413913	1824830	24.44%	3.371%

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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-BF110920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.557	2288	2290	2297	rVB	86247	109149	1.46%	0.202%
38	16.004	2361	2366	2371	rBV	57949	86627	1.16%	0.160%
39	16.074	2373	2378	2392	rVV8	59985	195178	2.61%	0.361%

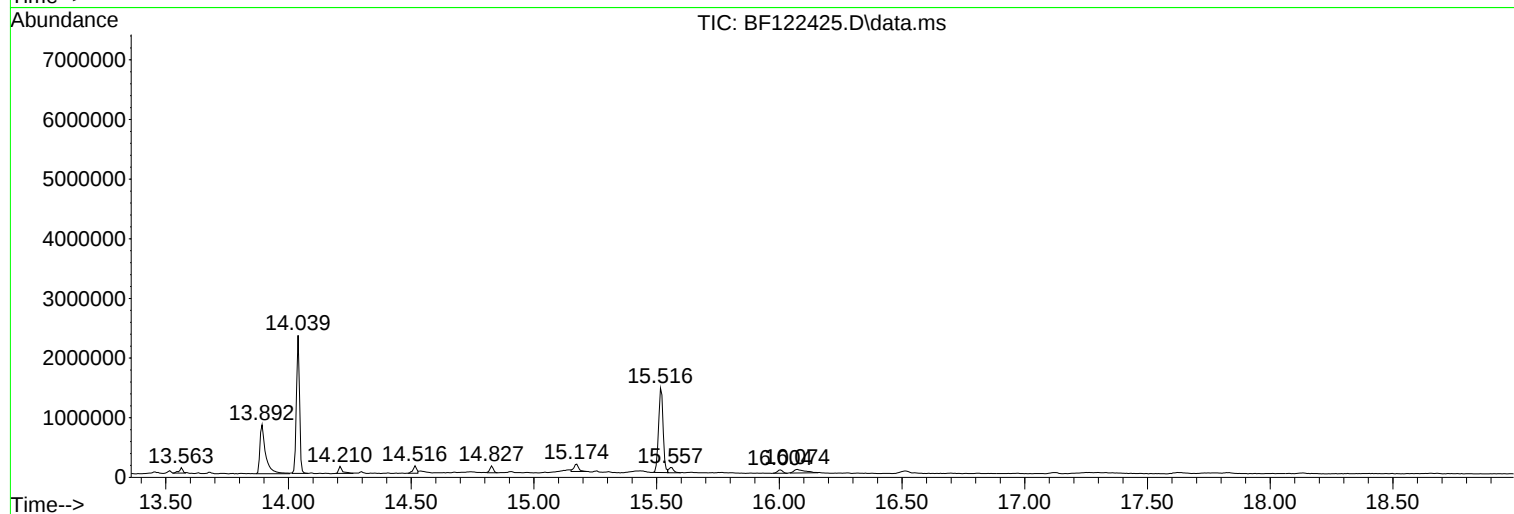
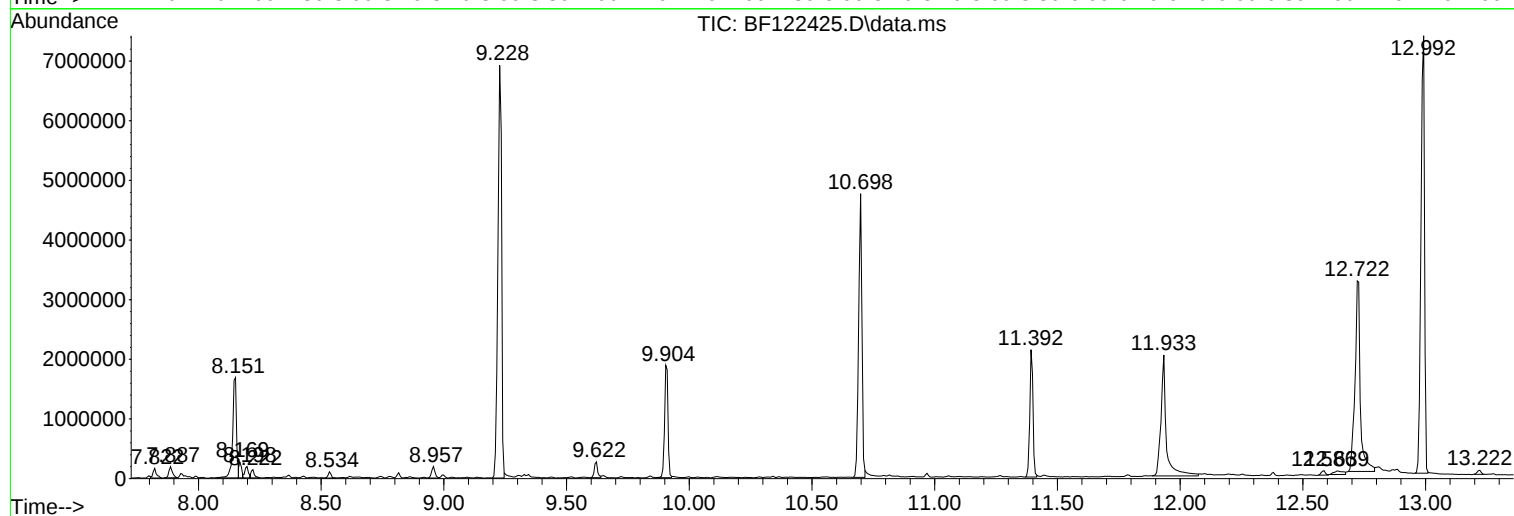
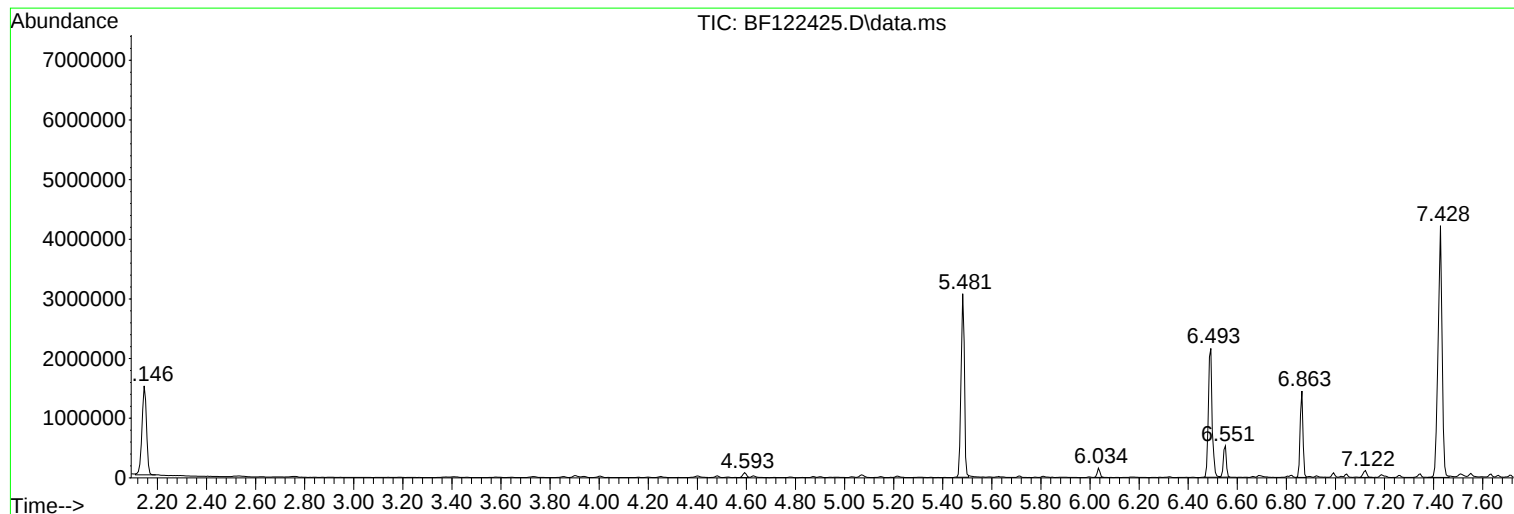
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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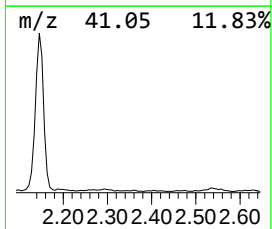
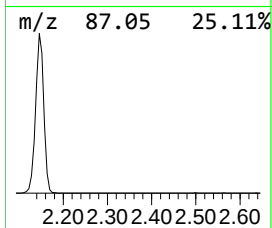
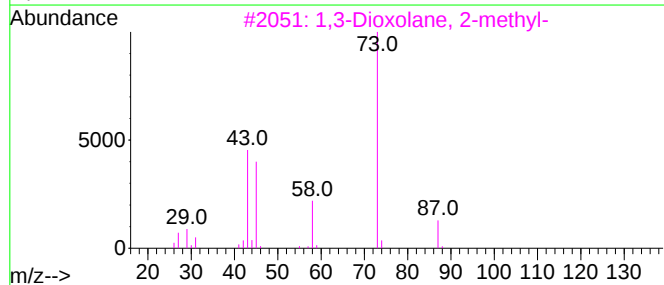
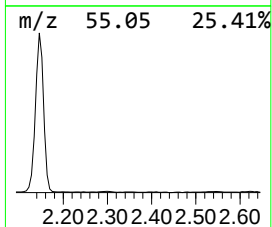
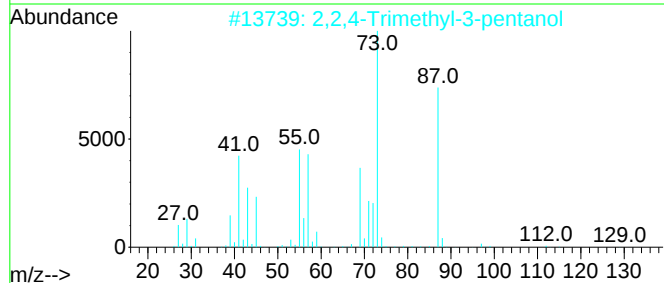
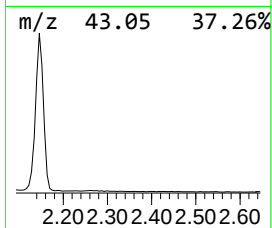
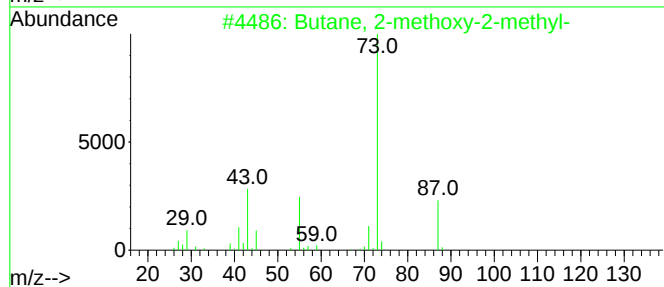
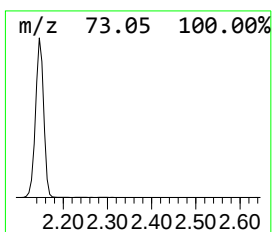
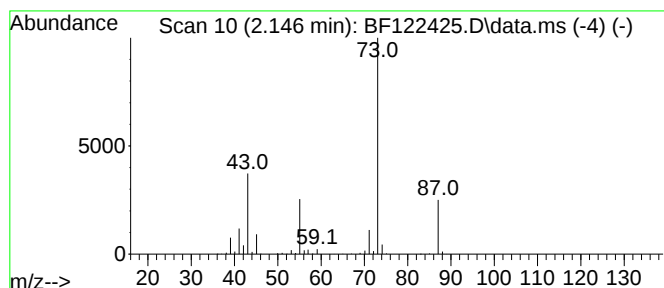
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	32.86 ng	1911000	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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Instrument :
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ClientSampleId :
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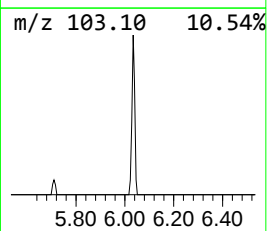
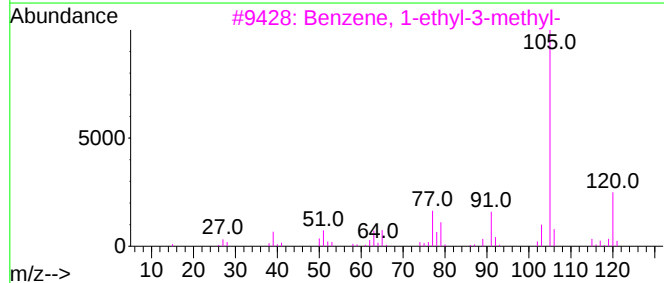
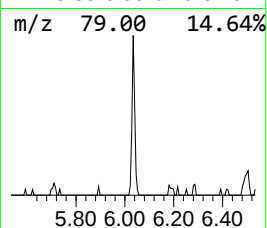
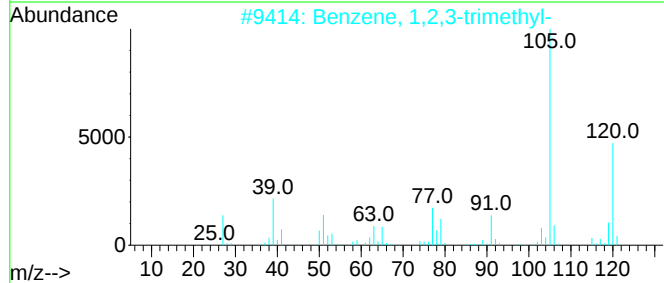
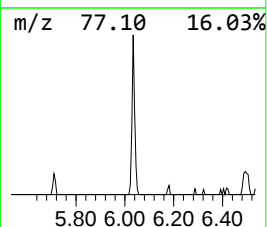
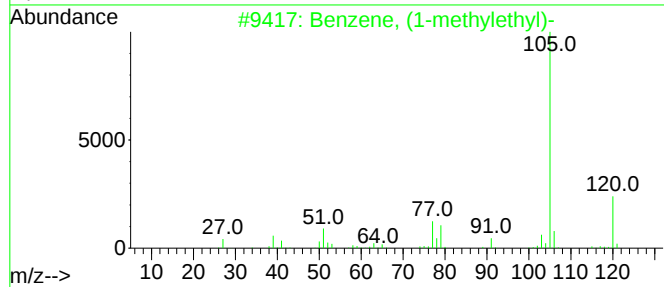
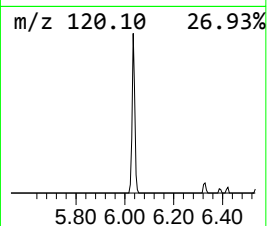
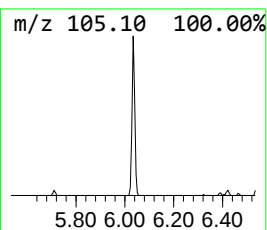
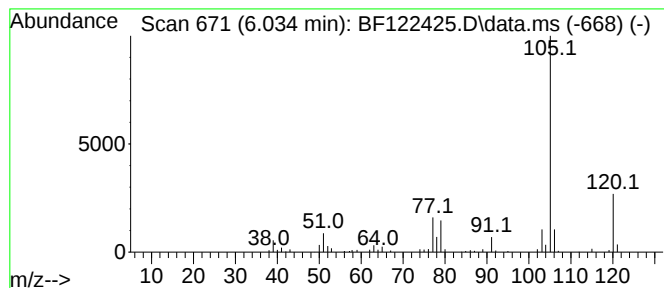
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, (1-methylethyl)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.034	2.12 ng	123367	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	94
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	80
4			2,3-Heptadien-5-yne, 2,4-dimethyl-	120	C9H12	041898-89-9	80
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	80



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Misc :
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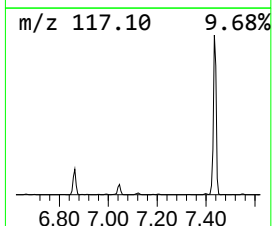
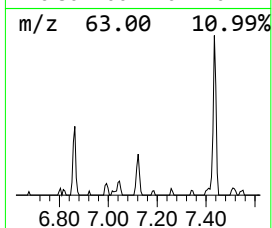
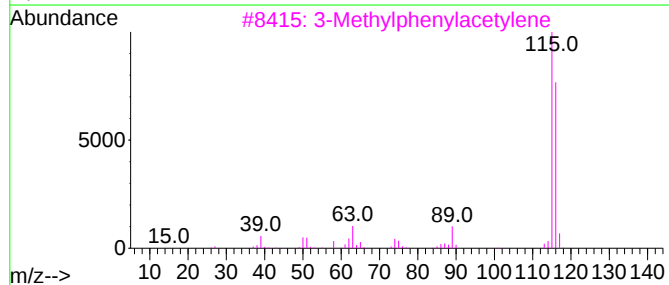
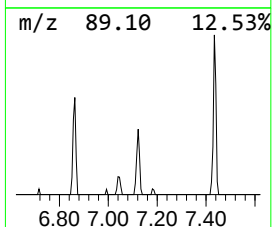
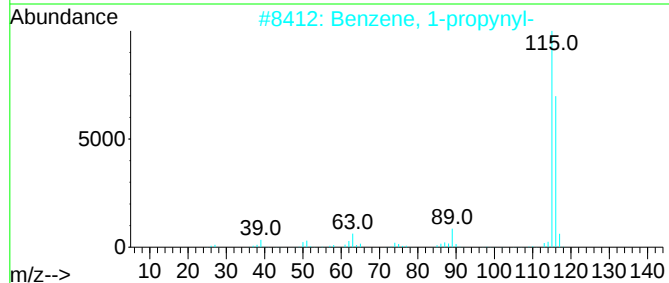
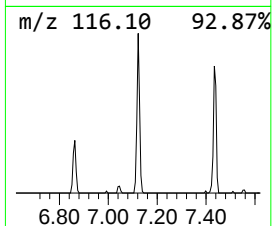
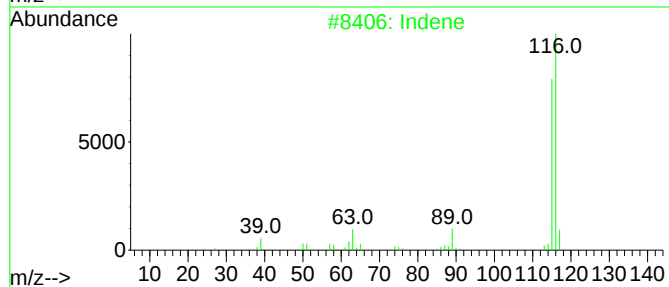
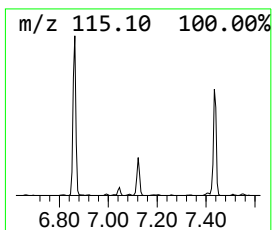
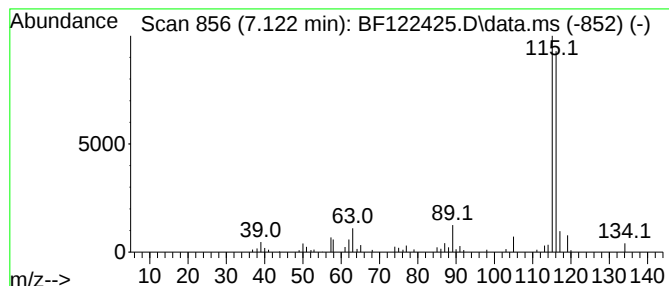
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Indene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.122	2.11 ng	122881	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	97
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90
5			2-Methylphenylacetylene	116	C9H8	000766-47-2	87



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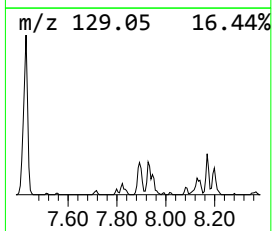
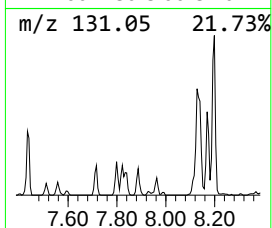
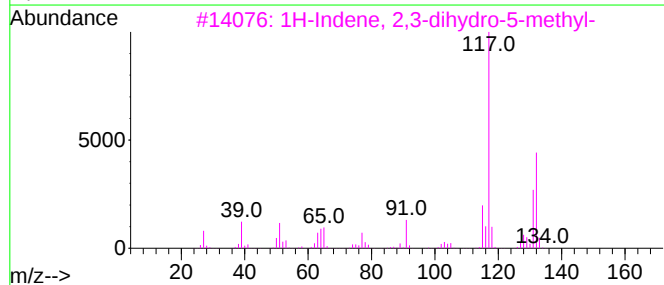
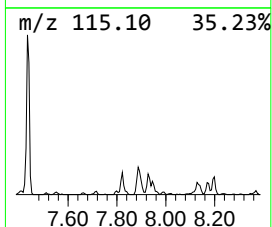
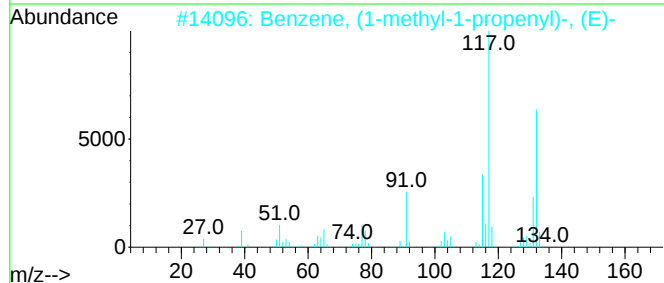
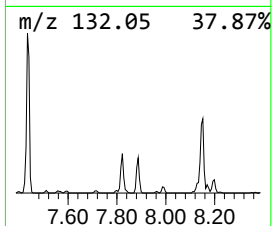
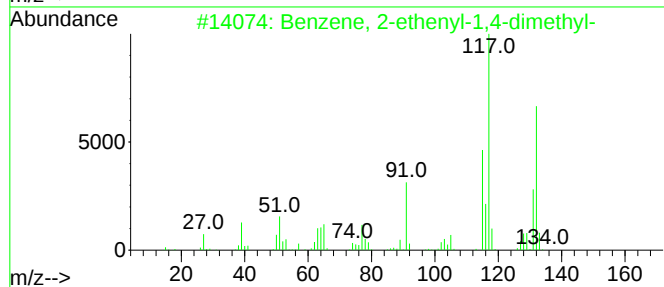
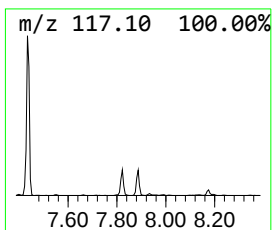
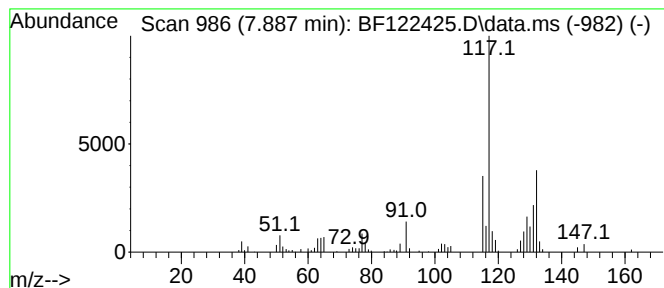
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.887	2.05 ng	187573	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	93
2			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	83
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	81
4			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	76
5			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	76



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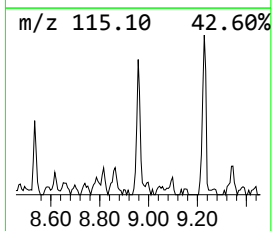
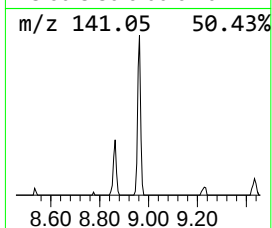
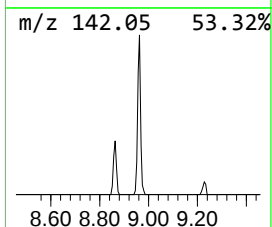
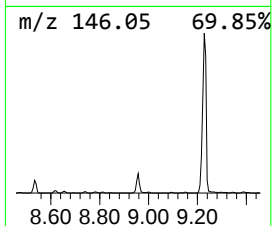
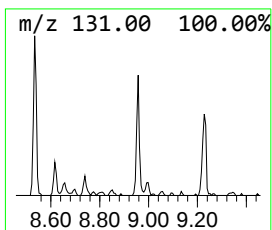
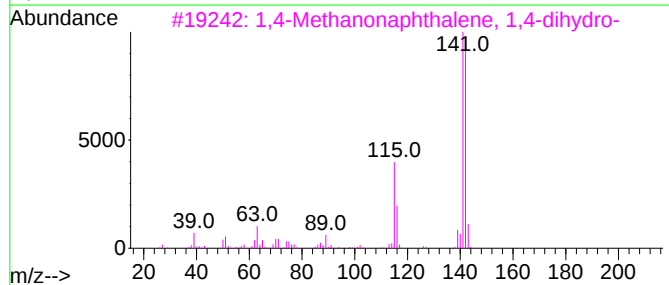
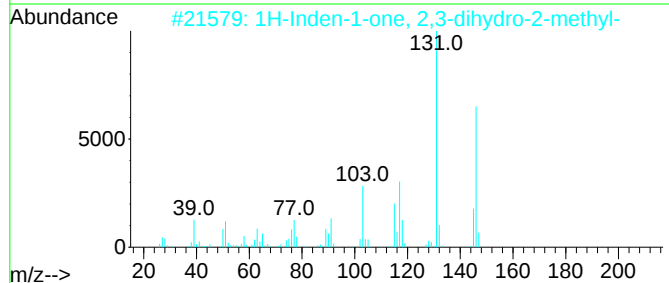
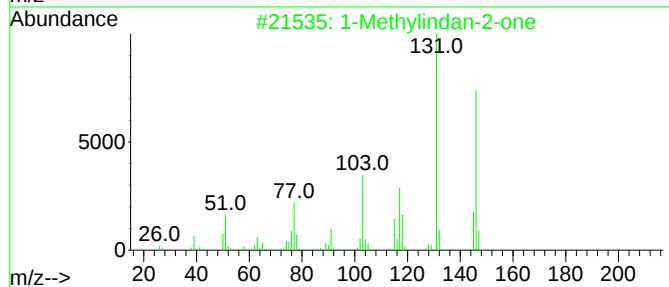
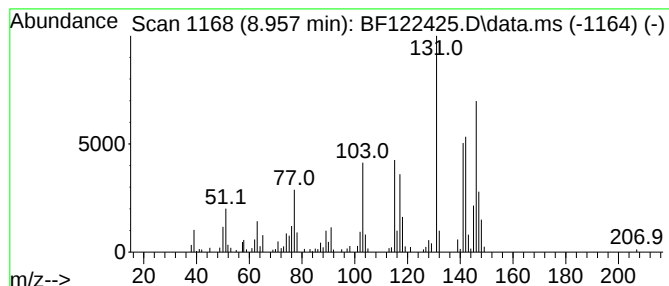
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Methylindan-2-one Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.957	2.01 ng	183215	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methylindan-2-one	146	C10H10O	035587-60-1	95
2			1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	64
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	52
4			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	49
5			1H-Inden-1-one, 2,3-dihydro-3-me...	146	C10H10O	006072-57-7	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
Data File : BF122425.D
Acq On : 21 Nov 2020 17:36
Operator : JU/CG
Sample : L4829-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

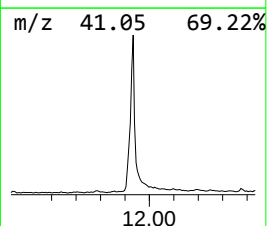
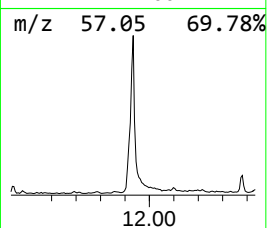
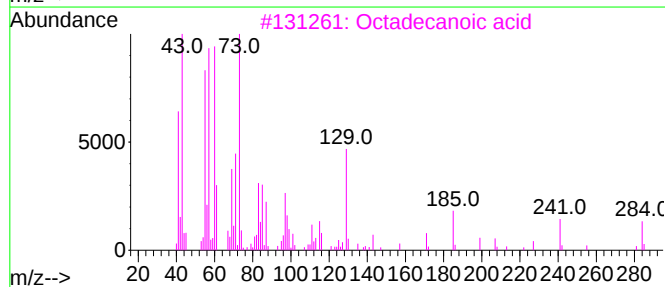
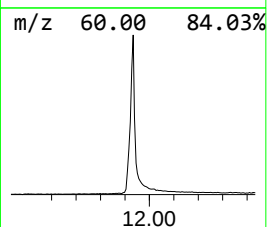
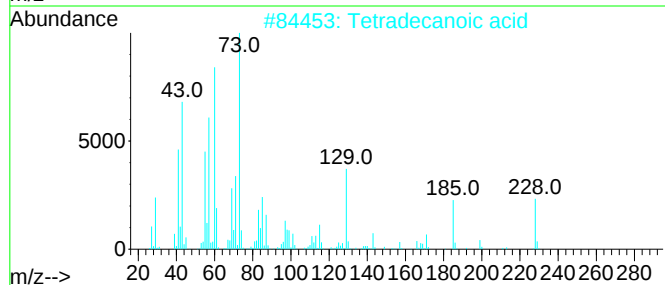
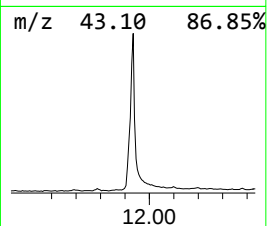
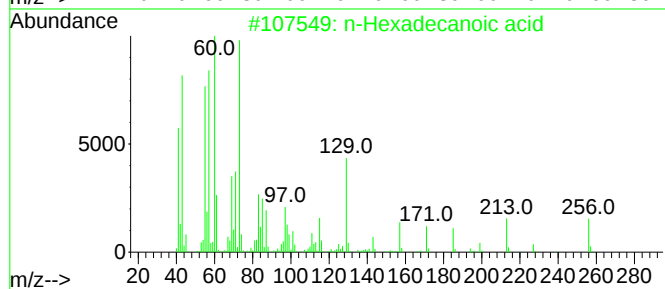
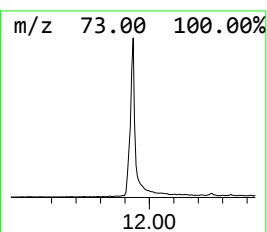
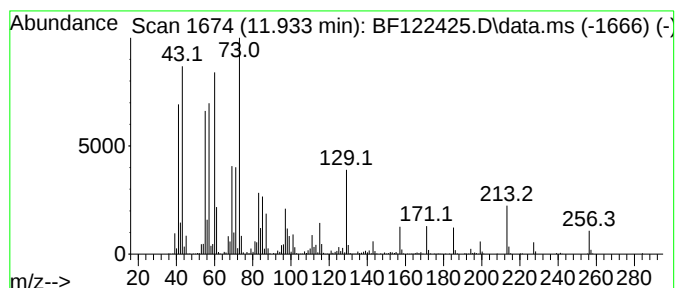
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.933	32.50 ng	3091850	Phenanthrene-d10	11.392	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Octadecanoic acid	284	C18H36O2	000057-11-4	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	Tridecanoic acid	214	C13H26O2	000638-53-9	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
Data File : BF122425.D
Acq On : 21 Nov 2020 17:36
Operator : JU/CG
Sample : L4829-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-9

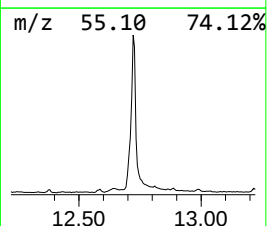
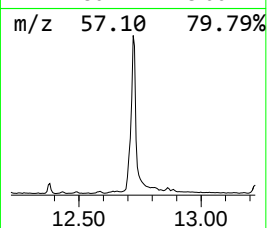
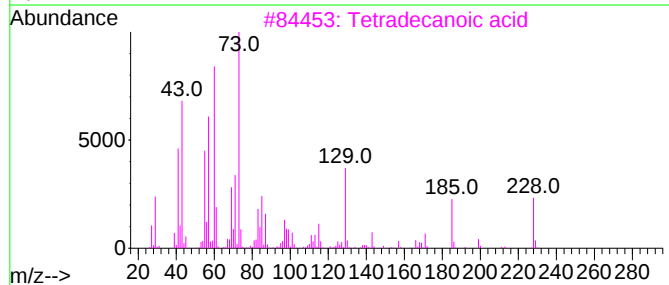
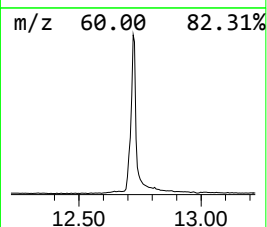
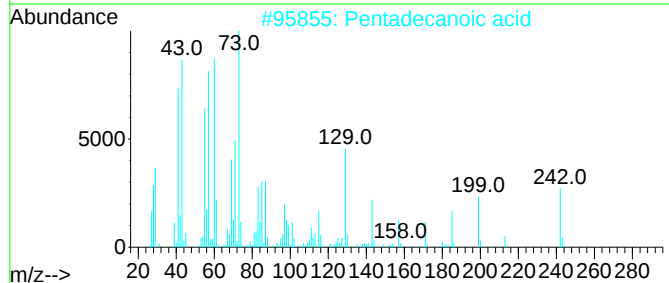
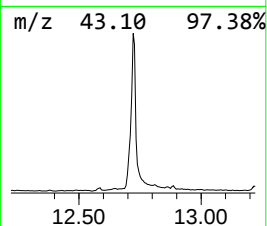
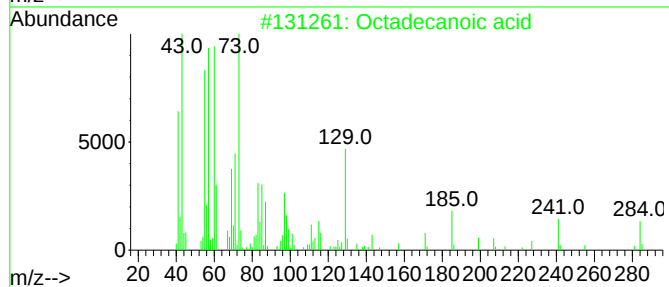
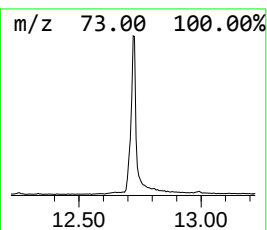
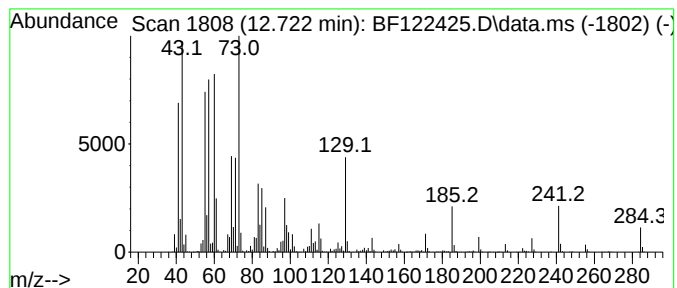
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.722	46.39 ng	4768190	Chrysene-d12	14.039

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	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5			Tridecanoic acid	214	C13H26O2	000638-53-9	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
Data File : BF122425.D
Acq On : 21 Nov 2020 17:36
Operator : JU/CG
Sample : L4829-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

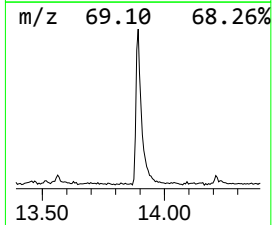
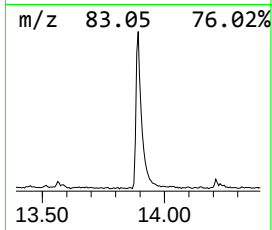
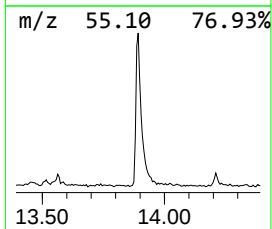
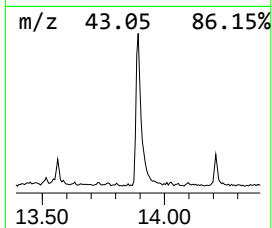
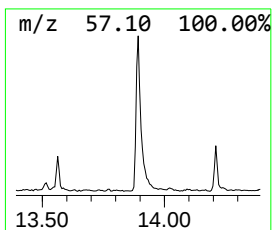
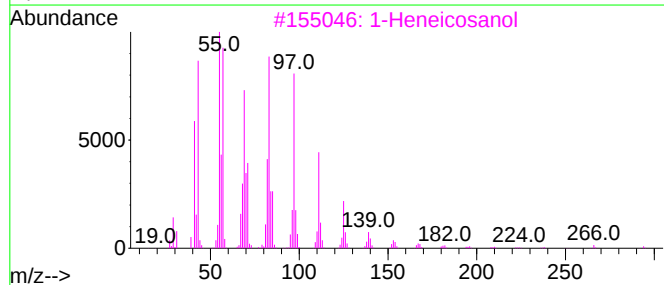
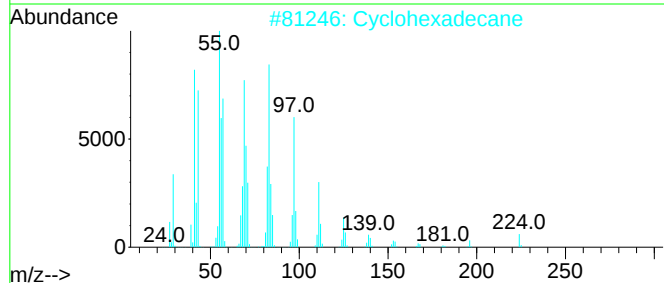
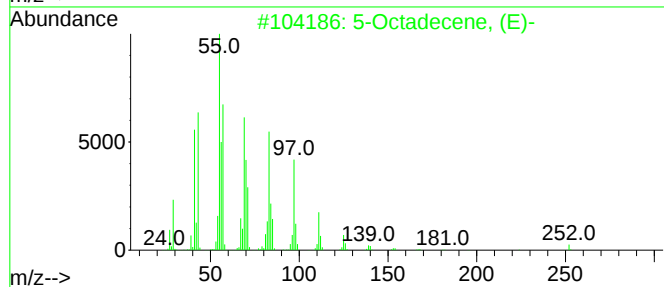
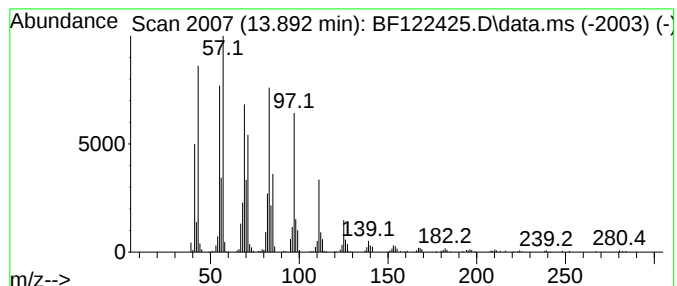
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 5-Octadecene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.892	12.90 ng	1325800	Chrysene-d12		14.039	
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-		252	C18H36	007206-21-5	95
2	Cyclohexadecane		224	C16H32	000295-65-8	95
3	1-Heneicosanol		312	C21H44O	015594-90-8	93
4	Octacosanol		410	C28H58O	000557-61-9	91
5	1-Heptacosanol		396	C27H56O	002004-39-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
Data File : BF122425.D
Acq On : 21 Nov 2020 17:36
Operator : JU/CG
Sample : L4829-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-9

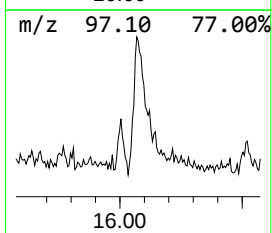
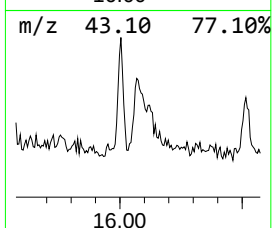
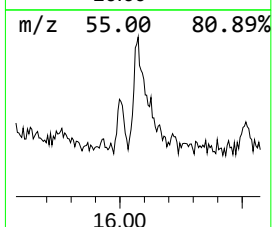
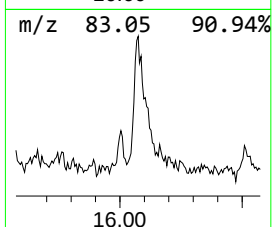
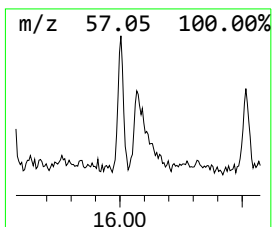
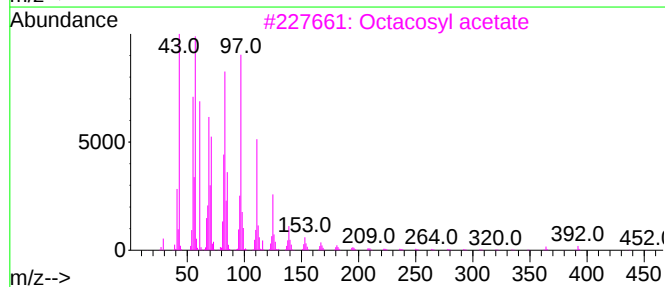
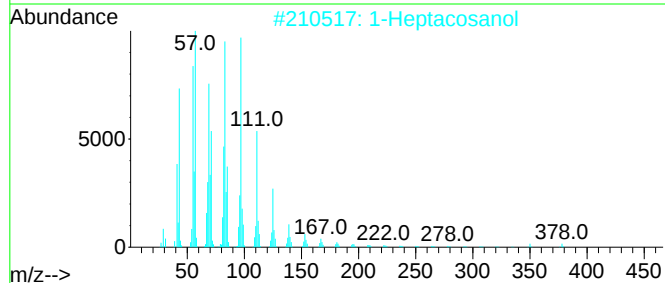
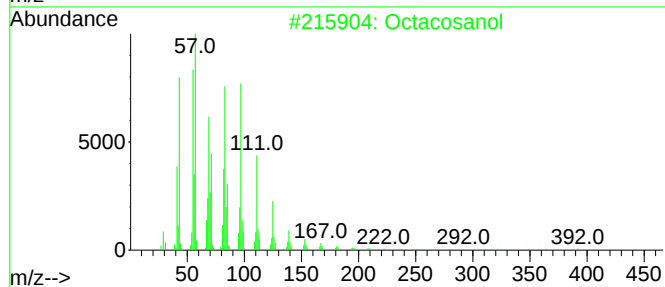
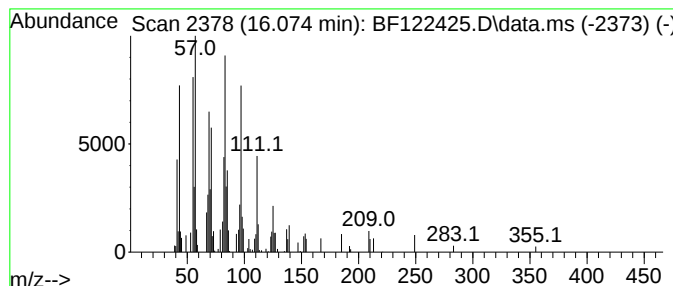
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Octacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.074	2.14 ng	195178	Perylene-d12	15.515

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosanol	410	C28H58O	000557-61-9	95
2		1-Heptacosanol	396	C27H56O	002004-39-9	95
3		Octacosyl acetate	452	C30H60O2	018206-97-8	95
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5		Behenic alcohol	326	C22H46O	000661-19-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
Data File : BF122425.D
Acq On : 21 Nov 2020 17:36
Operator : JU/CG
Sample : L4829-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.146	32.9	ng	1911000	1	6.863	1163080	20.0
Benzene, (1-met...	6.034	2.1	ng	123367	1	6.863	1163080	20.0
Indene	7.122	2.1	ng	122881	1	6.863	1163080	20.0
Benzene, 2-ethe...	7.887	2.0	ng	187573	2	8.151	1825850	20.0
1-Methylindan-2...	8.957	2.0	ng	183215	2	8.151	1825850	20.0
n-Hexadecanoic ...	11.933	32.5	ng	3091850	4	11.392	1902800	20.0
Octadecanoic acid	12.722	46.4	ng	4768190	5	14.039	2055520	20.0
5-Octadecene, (E)-	13.892	12.9	ng	1325800	5	14.039	2055520	20.0
Octacosanol	16.074	2.1	ng	195178	6	15.515	1824830	20.0