

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071222\
 Data File : BF129186.D
 Acq On : 12 Jul 2022 13:30
 Operator : CG\JU
 Sample : N3662-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20220495B-SIM/C1B-COMPOSITE

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-BF062922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129186.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.334	3	8	17	rVB	2847017	3777283	50.59%	6.419%
2	5.198	493	495	504	rVB	72674	94557	1.27%	0.161%
3	5.569	552	558	561	rBV	7154993	7175639	96.10%	12.194%
4	6.563	720	727	730	rBV	6326550	7466807	100.00%	12.689%
5	6.669	741	745	750	rBV	92326	104927	1.41%	0.178%
6	6.934	786	790	793	rVB	2163588	1797782	24.08%	3.055%
7	7.039	801	808	811	rBV6	36559	86667	1.16%	0.147%
8	7.198	830	835	840	rVB3	72409	87683	1.17%	0.149%
9	7.498	874	886	889	rBV	4672922	4832417	64.72%	8.212%
10	7.563	894	897	902	rBV4	57815	103753	1.39%	0.176%
11	8.216	1003	1008	1011	rBV	2635264	2330921	31.22%	3.961%
12	8.263	1014	1016	1019	rVB	157700	135312	1.81%	0.230%
13	8.298	1019	1022	1027	rVB4	56648	81359	1.09%	0.138%
14	8.416	1039	1042	1049	rVB5	74860	88483	1.19%	0.150%
15	8.498	1049	1056	1061	rBV4	95422	161025	2.16%	0.274%
16	8.628	1075	1078	1080	rBV	134955	114679	1.54%	0.195%
17	8.892	1120	1123	1127	rVB2	77100	86531	1.16%	0.147%
18	9.116	1159	1161	1165	rVB2	68323	78430	1.05%	0.133%
19	9.228	1178	1180	1185	rVB	173324	129232	1.73%	0.220%
20	9.292	1185	1191	1194	rBV	7330763	6976116	93.43%	11.855%
21	9.369	1200	1204	1207	rBV	113344	137127	1.84%	0.233%
22	9.551	1232	1235	1239	rBV3	64386	74934	1.00%	0.127%
23	9.628	1245	1248	1254	rVB4	67536	97006	1.30%	0.165%
24	9.680	1254	1257	1260	rBV2	317537	304989	4.08%	0.518%
25	9.833	1281	1283	1286	rBV	159499	138019	1.85%	0.235%
26	9.880	1286	1291	1294	rBV3	110292	139637	1.87%	0.237%
27	9.975	1301	1307	1310	rVB	2709825	2352701	31.51%	3.998%
28	10.004	1310	1312	1315	rBV	98097	87931	1.18%	0.149%
29	10.069	1321	1323	1328	rBV4	59111	83403	1.12%	0.142%
30	10.127	1329	1333	1335	rBV5	68649	94070	1.26%	0.160%
31	10.216	1345	1348	1352	rBV2	117888	141556	1.90%	0.241%
32	10.286	1357	1360	1362	rBV2	98077	105599	1.41%	0.179%
33	10.380	1372	1376	1381	rBV5	152848	191770	2.57%	0.326%
34	10.427	1381	1384	1386	rBV2	76858	85817	1.15%	0.146%
35	10.610	1412	1415	1418	rBV	303521	304720	4.08%	0.518%
36	10.669	1422	1425	1430	rBV5	68547	98097	1.31%	0.167%

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37	10.769	1434	1442	1445	rBV	4587578	4304192	57.64%	7.314%
38	10.880	1457	1461	1464	rBV2	449093	476377	6.38%	0.810%
39	11.345	1537	1540	1543	rBV	334069	340046	4.55%	0.578%
40	11.469	1557	1561	1563	rBV	2447509	2131108	28.54%	3.621%
41	11.492	1563	1565	1569	rVV	320771	288916	3.87%	0.491%
42	11.539	1571	1573	1576	rVB	115787	91706	1.23%	0.156%
43	11.698	1597	1600	1603	rBV2	155503	174039	2.33%	0.296%
44	11.980	1644	1648	1655	rBV3	453738	677240	9.07%	1.151%
45	12.521	1738	1740	1742	rVB	193138	147275	1.97%	0.250%
46	12.686	1765	1768	1770	rBV	506822	458401	6.14%	0.779%
47	12.721	1772	1774	1777	rVB2	217600	189314	2.54%	0.322%
48	12.916	1804	1807	1813	rVB	620865	607705	8.14%	1.033%
49	13.057	1827	1831	1834	rVB	5109406	4632328	62.04%	7.872%
50	13.239	1860	1862	1865	rVB	238087	214159	2.87%	0.364%
51	13.310	1872	1874	1877	rVB	192417	147526	1.98%	0.251%
52	14.115	2007	2011	2013	rBV2	1533768	1572222	21.06%	2.672%
53	14.139	2013	2015	2021	rVB	332780	315261	4.22%	0.536%
54	14.204	2024	2026	2031	rVB	540104	489993	6.56%	0.833%
55	15.562	2254	2257	2263	rVB	159589	228372	3.06%	0.388%
56	15.627	2264	2268	2277	rVB	883473	1213662	16.25%	2.062%

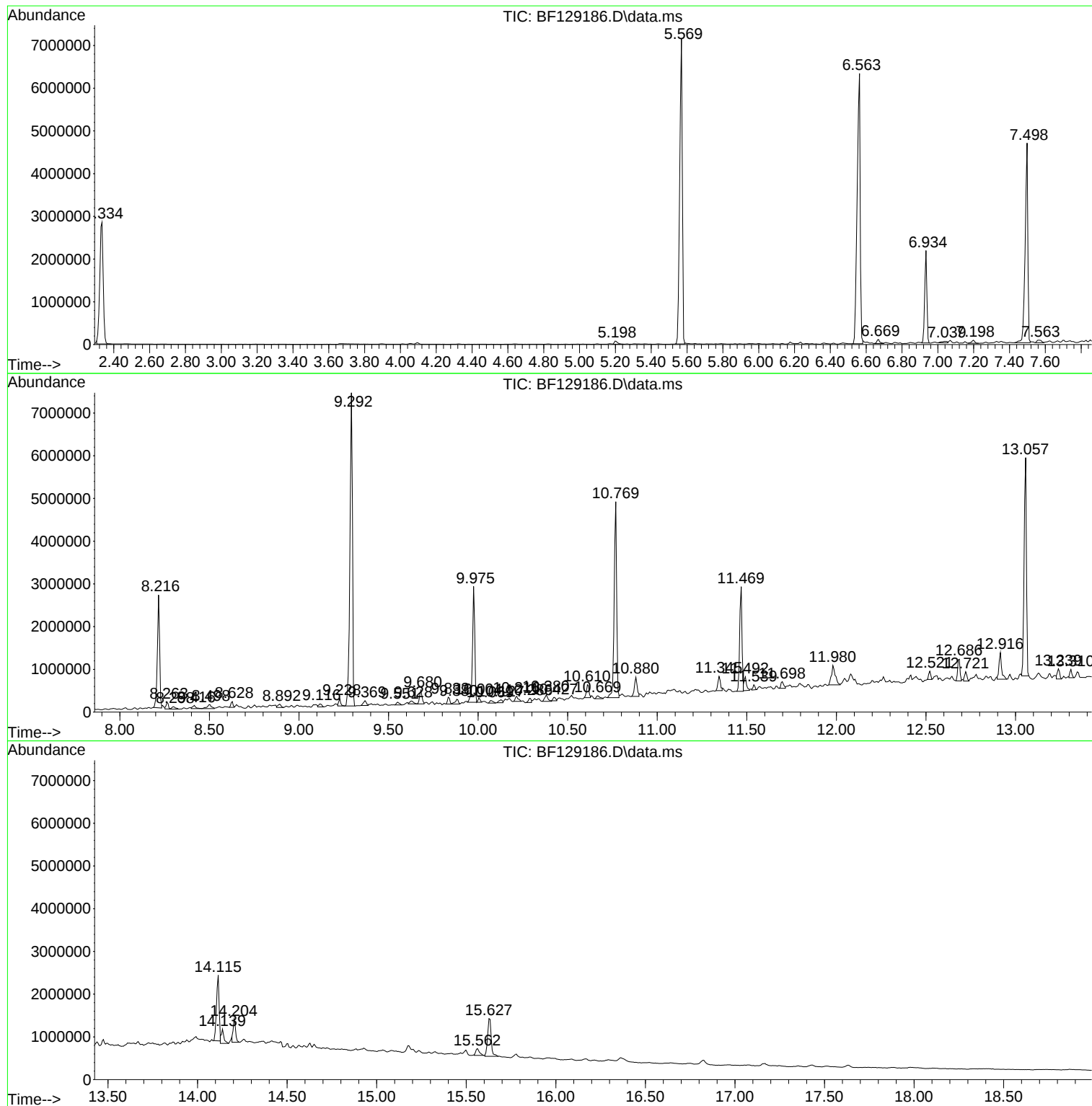
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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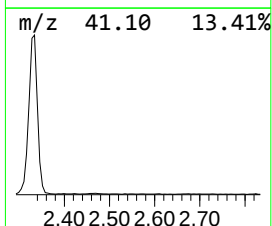
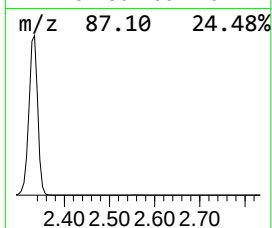
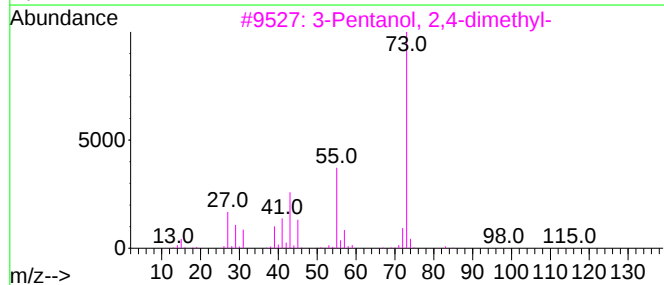
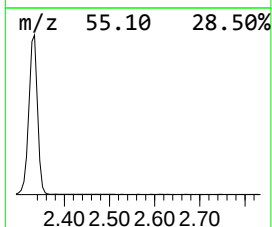
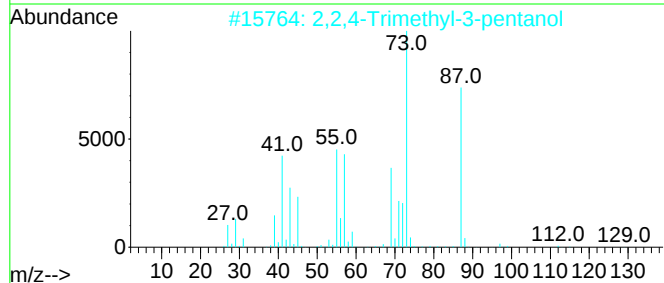
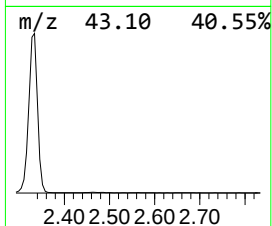
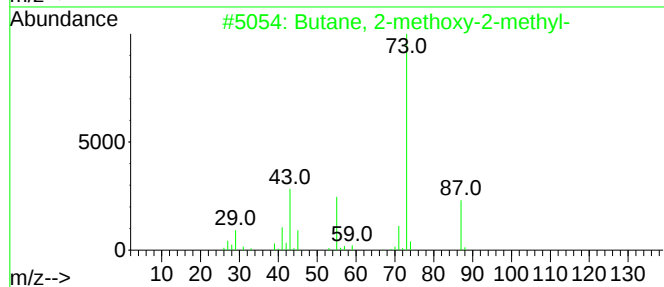
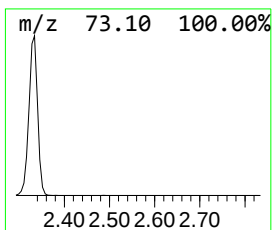
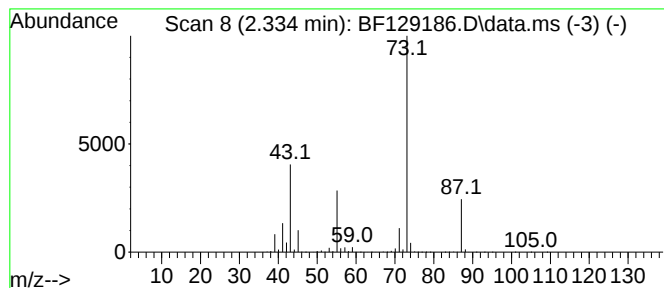
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.334	42.02 ng	3777280	1,4-Dichlorobenzene-d4	6.934

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			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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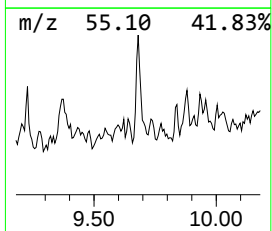
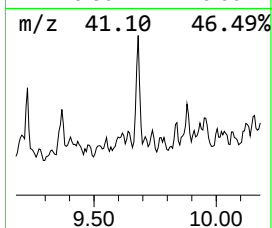
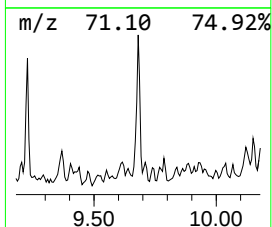
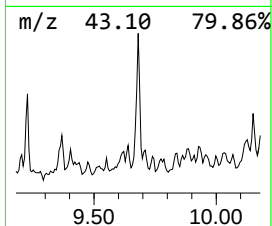
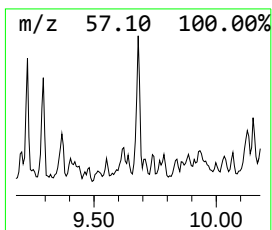
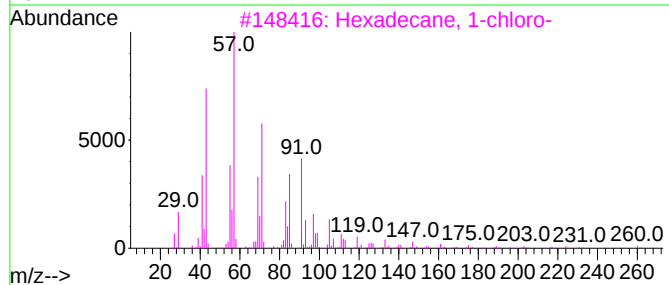
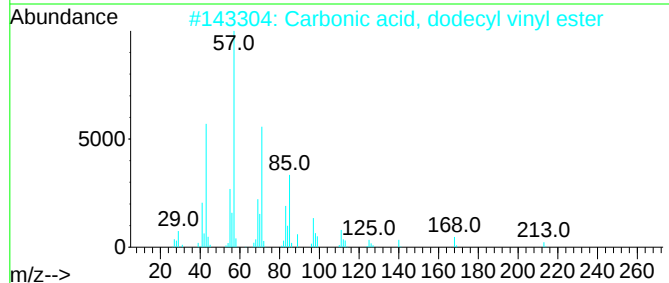
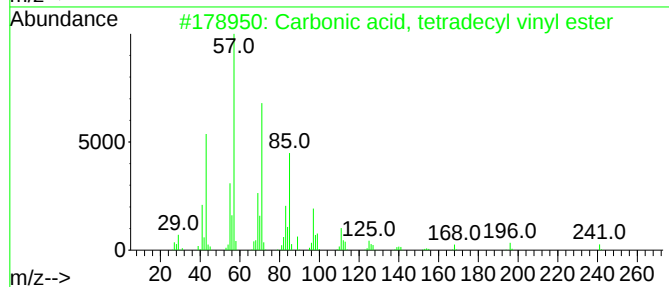
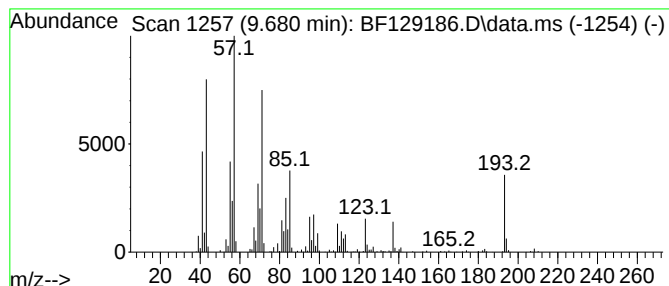
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Carbonic acid, tetradecyl v... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.680	2.59 ng	304989	Acenaphthene-d10	9.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	52
2			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	52
3			Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	52
4			Carbonic acid, tridecyl vinyl ester	270	C16H30O3	1000382-54-7	52
5			1,3-Dimethylcyclopentanol	114	C7H14O	019550-46-0	49



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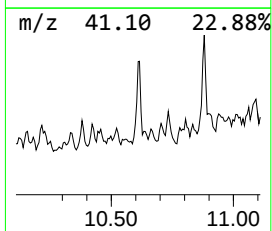
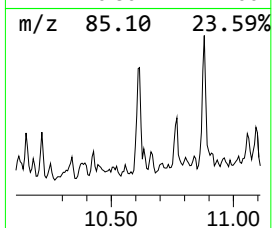
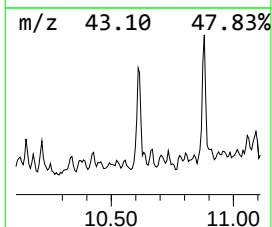
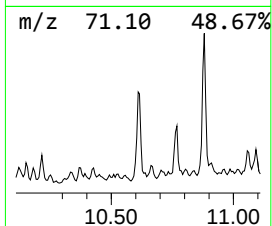
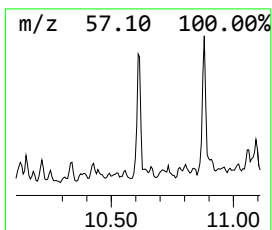
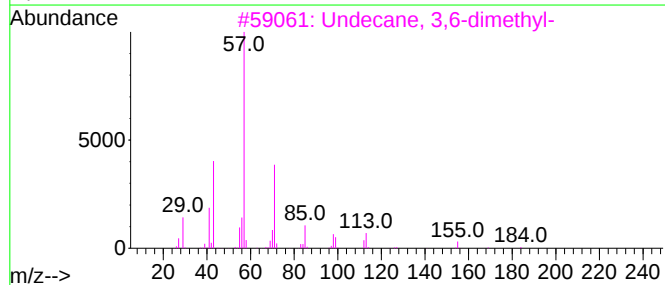
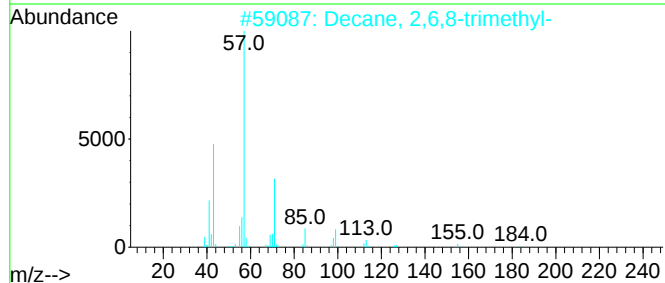
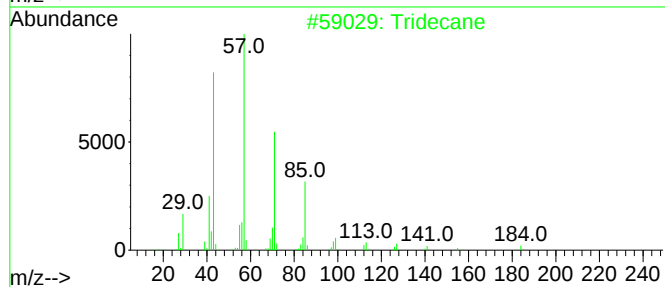
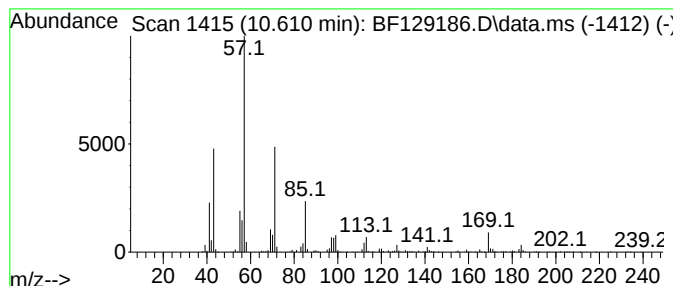
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Tridecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	2.59 ng	304720	Acenaphthene-d10	9.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	72
2			Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	68
3			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	59
4			Octacosane	394	C28H58	000630-02-4	58
5			Tetracosane	338	C24H50	000646-31-1	58



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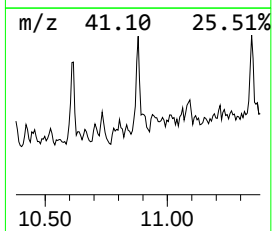
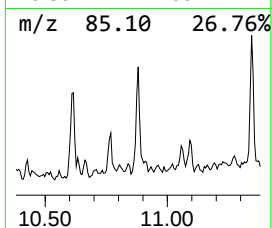
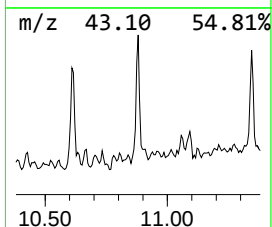
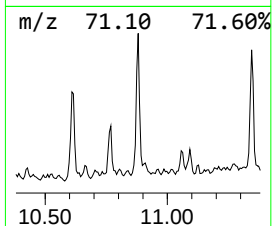
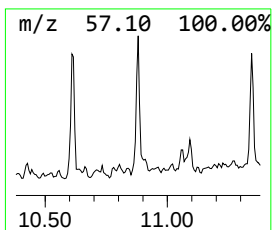
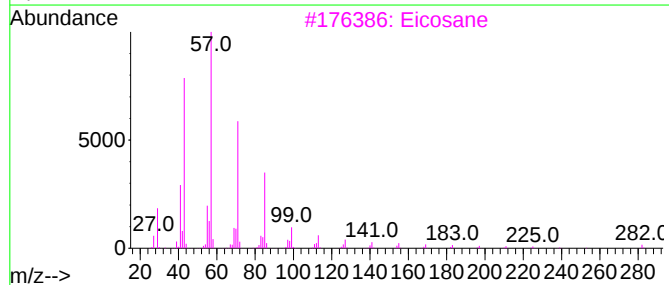
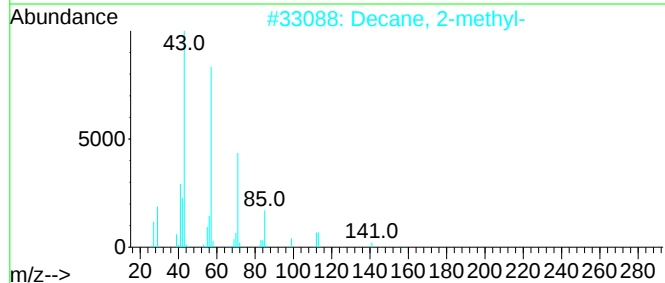
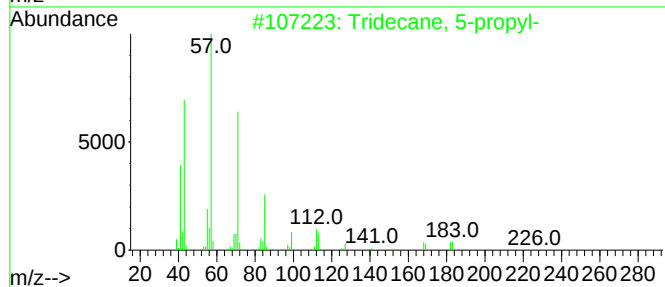
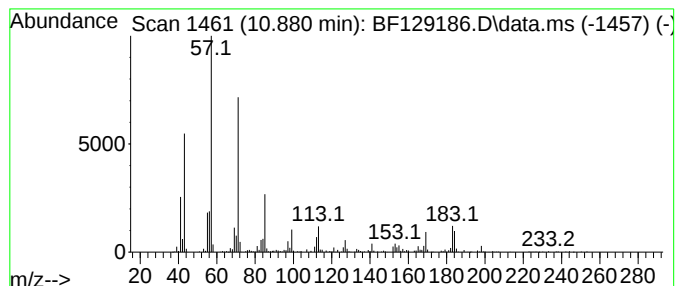
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tridecane, 5-propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.880	4.47 ng	476377	Phenanthrene-d10	11.469

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 5-propyl-	226	C16H34	055045-11-9	81
2			Decane, 2-methyl-	156	C11H24	006975-98-0	68
3			Eicosane	282	C20H42	000112-95-8	64
4			Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	64
5			3-Ethyl-2,6,10-trimethylundecane	226	C16H34	1000432-25-9	58



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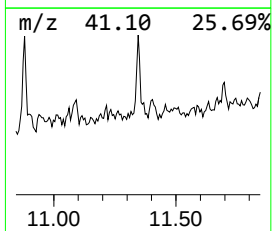
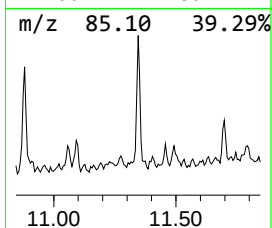
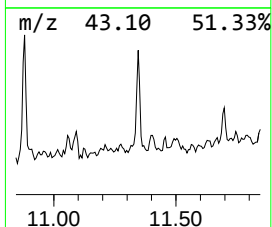
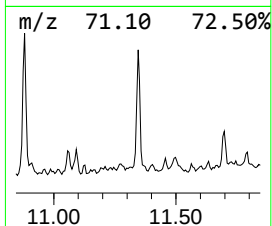
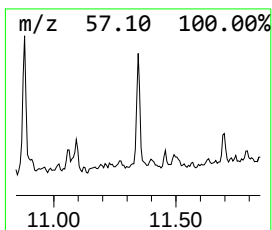
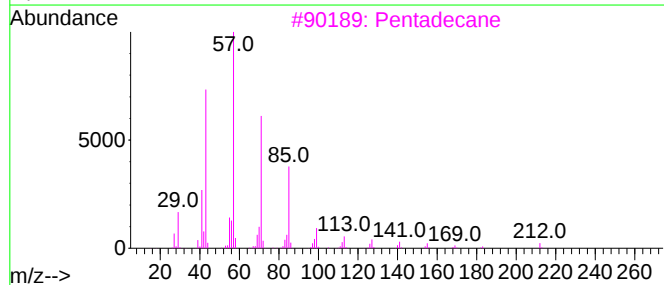
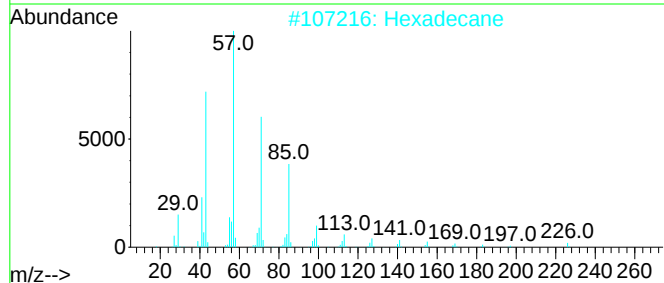
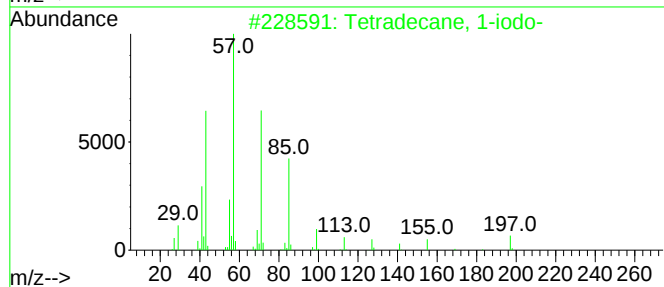
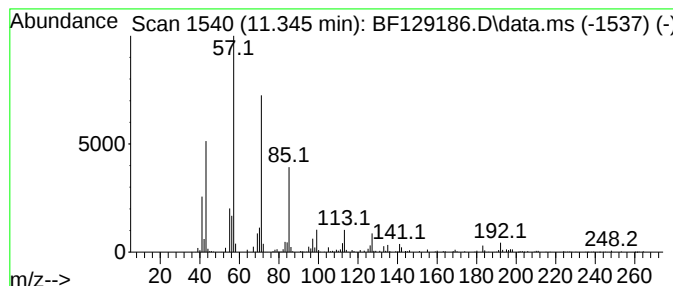
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tetradecane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.345	3.19 ng	340046	Phenanthrene-d10	11.469

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	90
2			Hexadecane	226	C16H34	000544-76-3	87
3			Pentadecane	212	C15H32	000629-62-9	86
4			Heptacosane	380	C27H56	000593-49-7	86
5			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071222\
Data File : BF129186.D
Acq On : 12 Jul 2022 13:30
Operator : CG\JU
Sample : N3662-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220495B-SIM/C1B-COMPOSITE

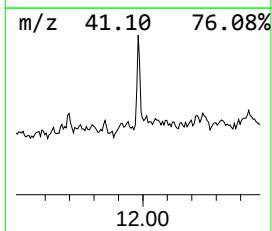
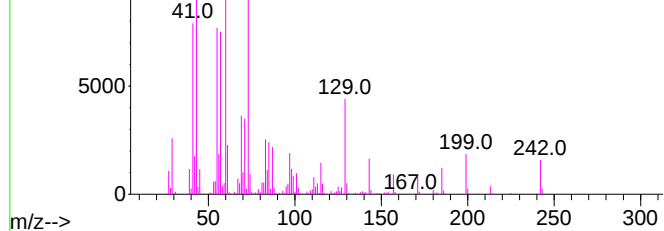
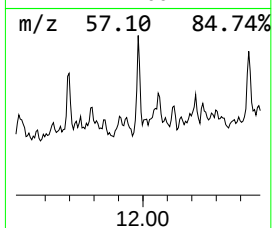
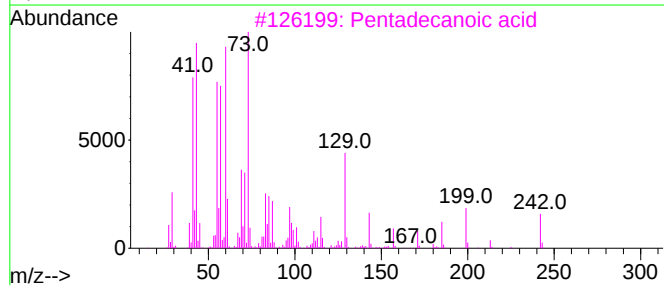
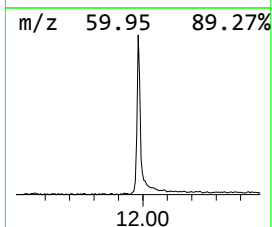
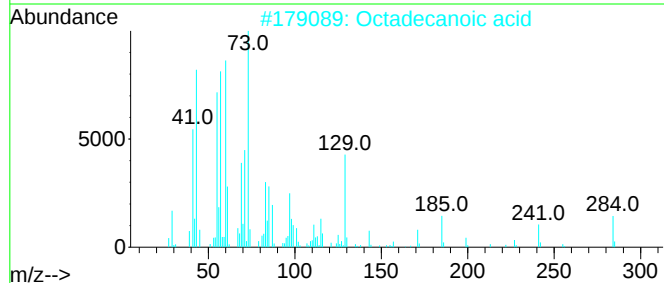
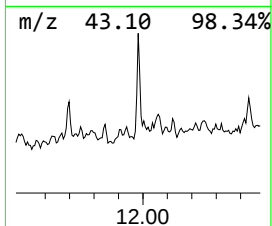
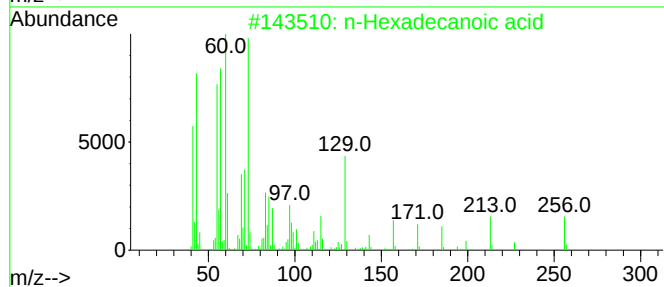
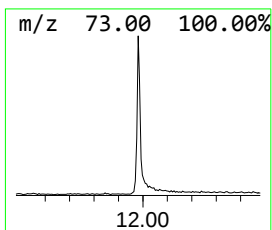
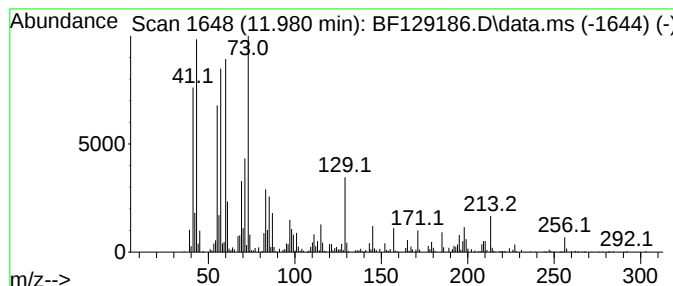
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.980	6.36 ng	677240	Phenanthrene-d10	11.469

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	96
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			Tridecanoic acid	214	C13H26O2	000638-53-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071222\
Data File : BF129186.D
Acq On : 12 Jul 2022 13:30
Operator : CG\JU
Sample : N3662-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220495B-SIM/C1B-COMPOSITE

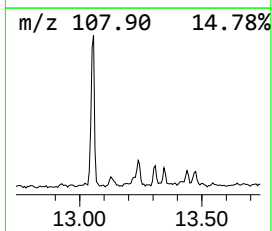
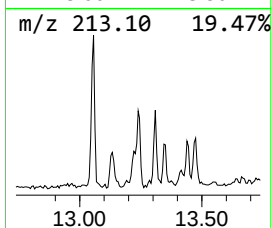
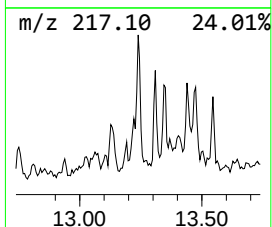
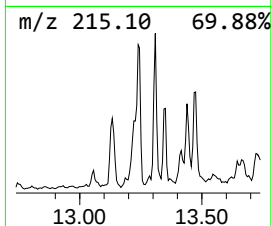
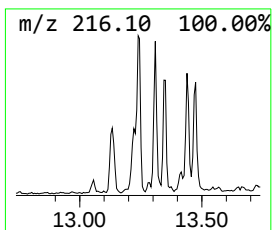
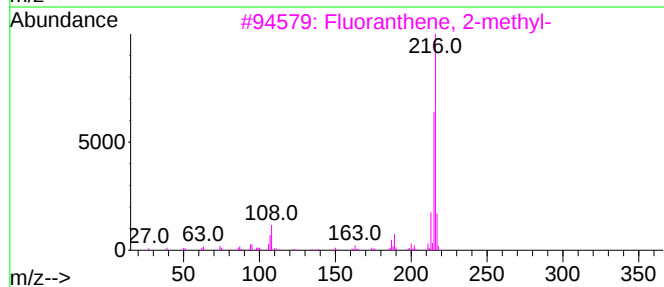
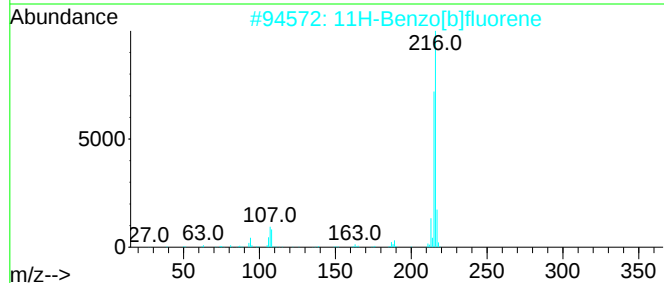
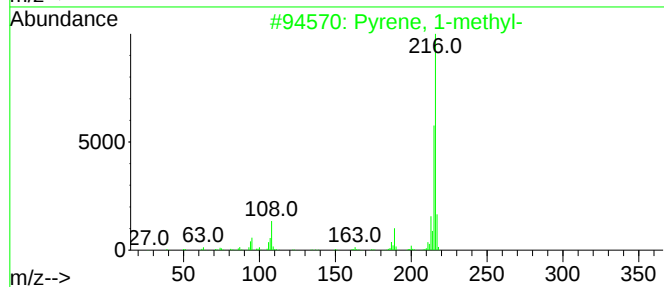
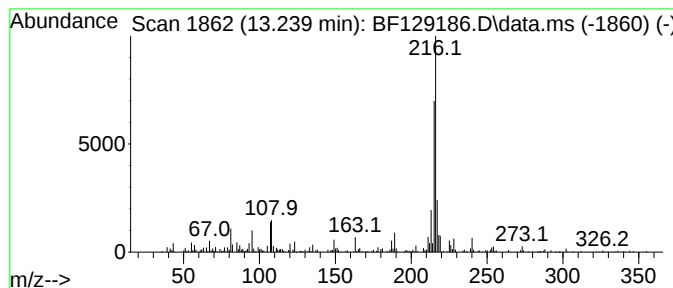
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pyrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.239	2.72 ng	214159	Chrysene-d12	14.115

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
2			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	83
3			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	81
4			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	80
5			Pyrene, 2-methyl-	216	C17H12	003442-78-2	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071222\
Data File : BF129186.D
Acq On : 12 Jul 2022 13:30
Operator : CG\JU
Sample : N3662-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
20220495B-SIM/C1B-COMPOSITE

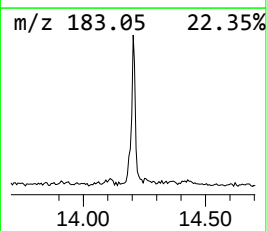
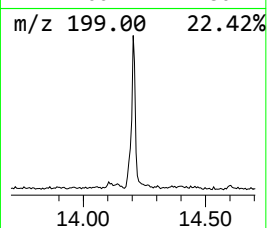
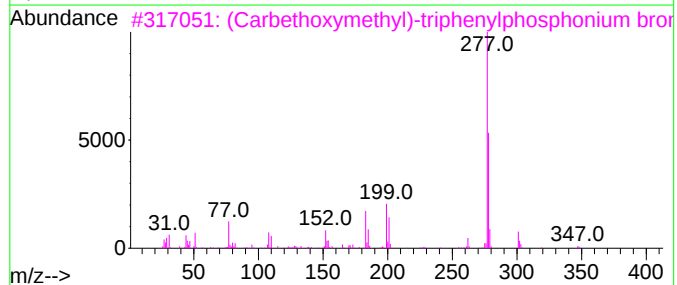
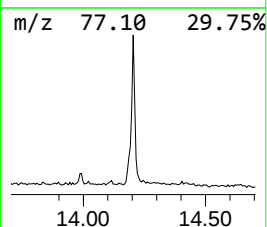
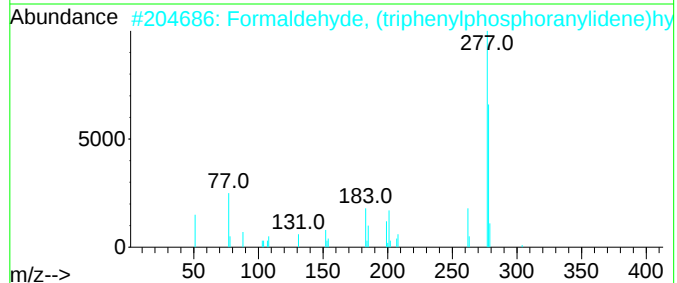
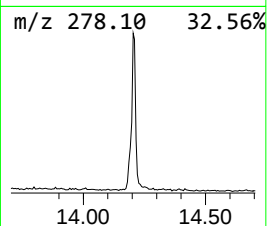
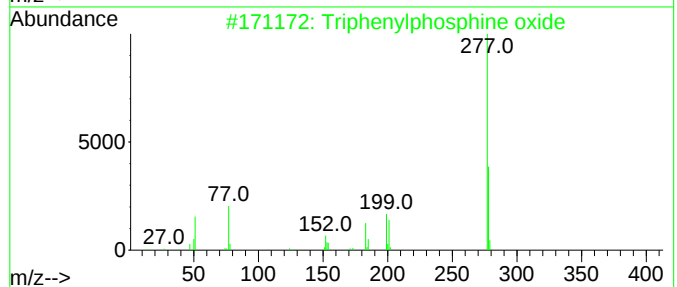
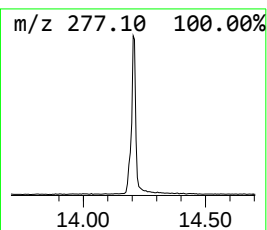
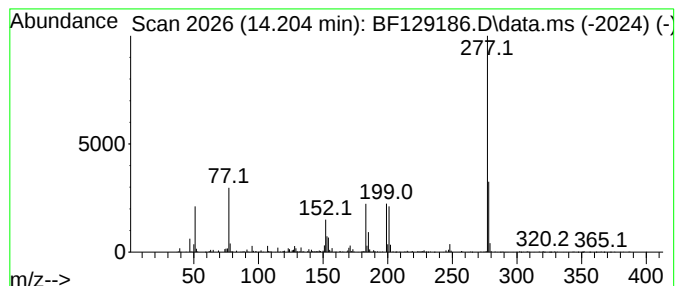
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.204	6.23 ng	489993	Chrysene-d12	14.115

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
3			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	50
4			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19N03S	1000483-83-4	49
5			4-Nitro-4'-methyldiphenylsulfone	277	C13H11N04S	004094-37-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071222\
Data File : BF129186.D
Acq On : 12 Jul 2022 13:30
Operator : CG\JU
Sample : N3662-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220495B-SIM/C1B-COMPOSITE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.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
Butane, 2-metho...	2.334	42.0	ng	3777280	1	6.934	1797780	20.0
Carbonic acid, ...	9.680	2.6	ng	304989	3	9.975	2352700	20.0
Tridecane	10.610	2.6	ng	304720	3	9.975	2352700	20.0
Tridecane, 5-pr...	10.880	4.5	ng	476377	4	11.469	2131110	20.0
Tetradecane, 1-...	11.345	3.2	ng	340046	4	11.469	2131110	20.0
n-Hexadecanoic ...	11.980	6.4	ng	677240	4	11.469	2131110	20.0
Pyrene, 1-methyl-	13.239	2.7	ng	214159	5	14.115	1572220	20.0
Triphenylphosph...	14.204	6.2	ng	489993	5	14.115	1572220	20.0