

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110920\
 Data File : BP003885.D
 Acq On : 10 Nov 2020 03:35
 Operator : CG/JU
 Sample : L4668-01
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 MW-18

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_P\METHODS\8270-BP110320.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003885.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.099	29	36	47	rBV	196883	452009	5.45%	0.966%
2	3.193	47	52	69	rVB	1015990	1507048	18.17%	3.222%
3	5.822	493	499	512	rBV	1538107	2377217	28.66%	5.083%
4	7.469	771	779	790	rBV	909620	1529724	18.44%	3.271%
5	8.305	912	921	928	rVB	776045	1219956	14.71%	2.608%
6	8.699	982	988	998	rVB	77238	128968	1.55%	0.276%
7	9.469	1106	1119	1125	rBV	2396131	4027713	48.56%	8.611%
8	9.522	1125	1128	1138	rVB2	46100	96978	1.17%	0.207%
9	9.963	1198	1203	1208	rVB3	58947	94214	1.14%	0.201%
10	10.540	1295	1301	1308	rBV3	57954	99475	1.20%	0.213%
11	11.134	1395	1402	1408	rBV	955528	1623452	19.57%	3.471%
12	11.722	1497	1502	1510	rVB2	52003	96145	1.16%	0.206%
13	12.228	1582	1588	1594	rVB	136477	233954	2.82%	0.500%
14	12.451	1616	1626	1630	rBV3	40095	96950	1.17%	0.207%
15	12.593	1639	1650	1654	rBV7	37154	113360	1.37%	0.242%
16	12.669	1657	1663	1668	rVB	128408	200653	2.42%	0.429%
17	12.987	1707	1717	1727	rBV2	261437	543938	6.56%	1.163%
18	13.381	1779	1784	1790	rVB4	45517	90903	1.10%	0.194%
19	13.546	1804	1812	1819	rBV	5643506	8294786	100.00%	17.734%
20	13.928	1873	1877	1882	rVB3	73759	102641	1.24%	0.219%
21	14.240	1926	1930	1942	rBV3	112677	244947	2.95%	0.524%
22	14.345	1943	1948	1952	rVB	173434	239455	2.89%	0.512%
23	14.510	1973	1976	1983	rVB2	72997	114828	1.38%	0.246%
24	14.645	1995	1999	2005	rVB	87183	125262	1.51%	0.268%
25	14.922	2040	2046	2052	rVV	1342167	1983109	23.91%	4.240%
26	14.981	2053	2056	2063	rVB2	65779	97275	1.17%	0.208%
27	15.310	2108	2112	2118	rVB	56671	94652	1.14%	0.202%
28	15.534	2146	2150	2156	rVB6	76952	143738	1.73%	0.307%
29	15.598	2157	2161	2165	rBV4	63404	104052	1.25%	0.222%
30	15.951	2218	2221	2227	rVB2	91337	132539	1.60%	0.283%
31	16.087	2240	2244	2248	rBV2	104456	141189	1.70%	0.302%
32	16.275	2272	2276	2284	rBV2	201686	403358	4.86%	0.862%
33	16.404	2292	2298	2311	rVB	3746473	5527514	66.64%	11.818%
34	17.651	2505	2510	2515	rVB	1367157	1866719	22.50%	3.991%
35	18.492	2649	2653	2659	rBV	385898	582532	7.02%	1.245%
36	20.145	2928	2934	2939	rVB	6093735	7495190	90.36%	16.025%

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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_P\METHODS\8270-BP110320.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.327	3131	3135	3146	rVB	901805	1138038	13.72%	2.433%
38	21.674	3189	3194	3204	rVB	1266364	1714498	20.67%	3.666%
39	24.157	3609	3616	3628	rVB	814539	1693537	20.42%	3.621%

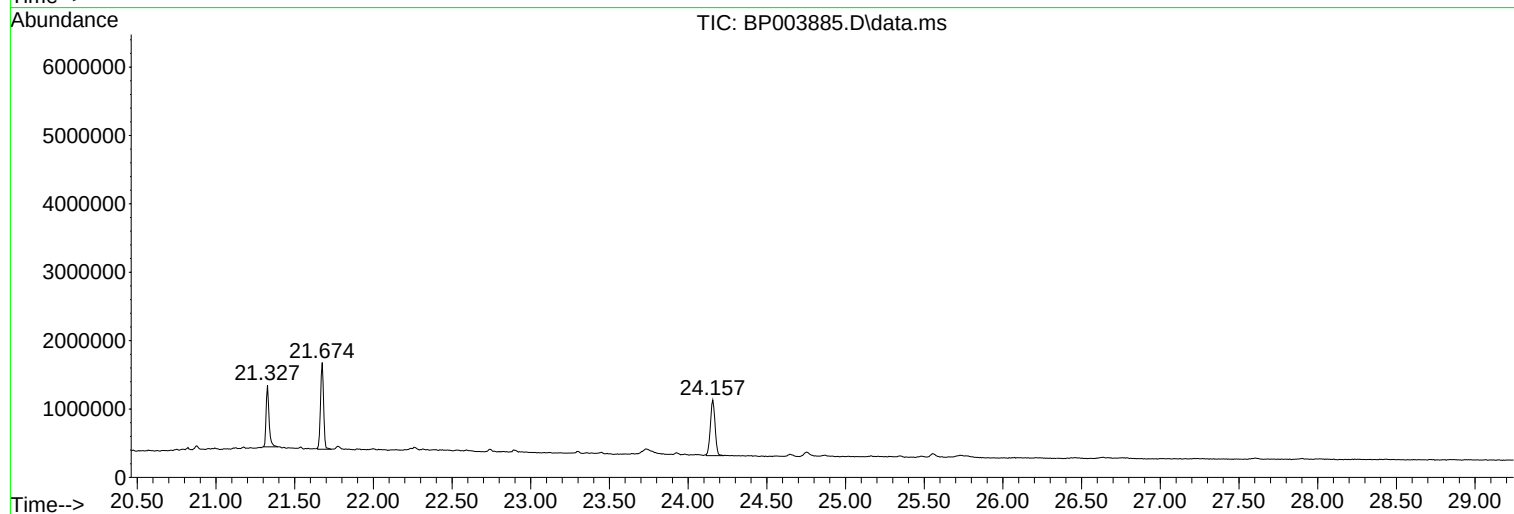
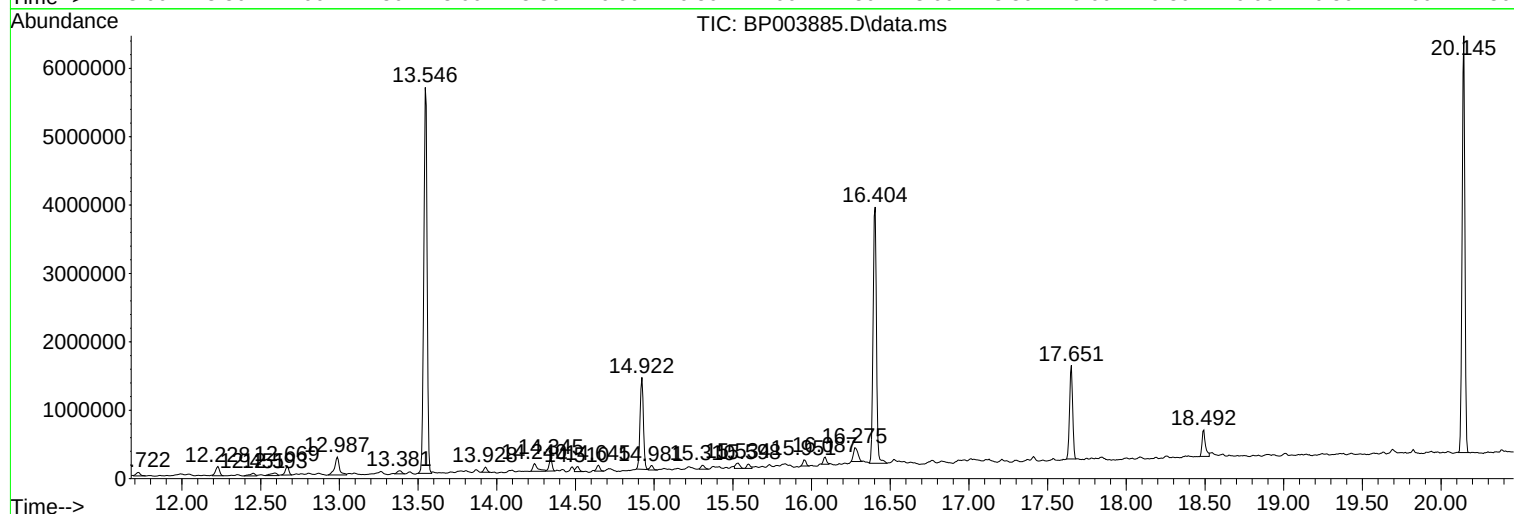
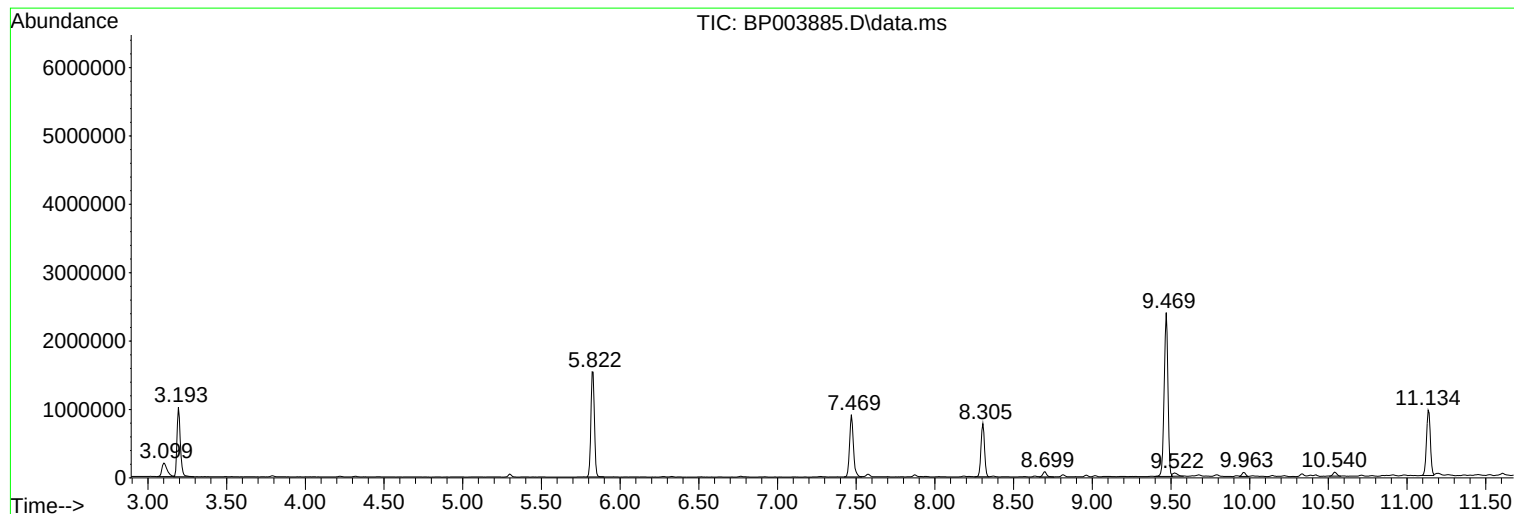
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : CG/JU
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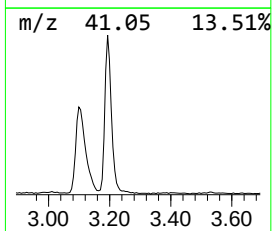
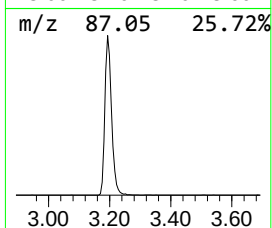
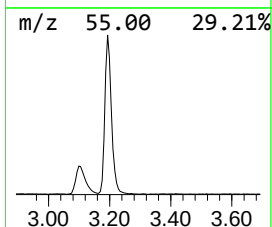
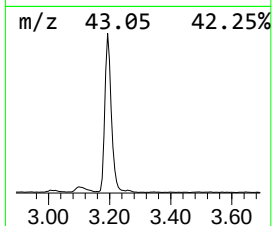
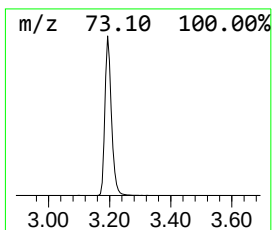
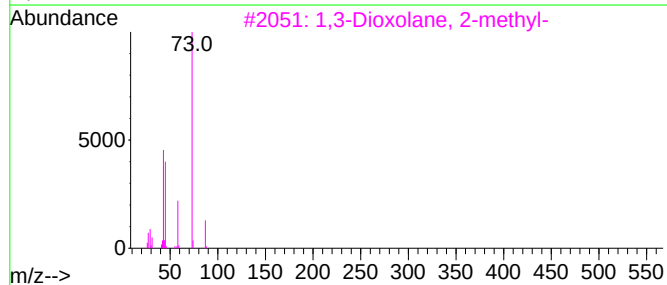
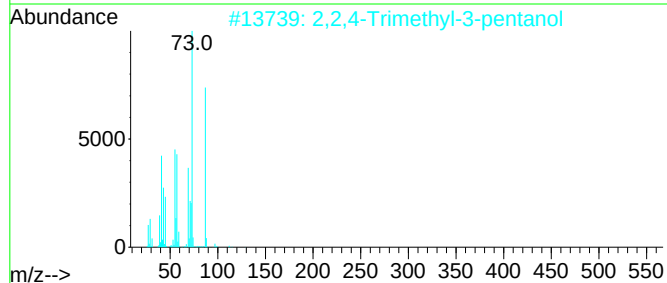
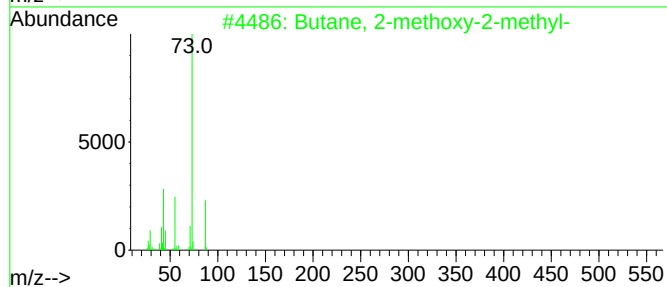
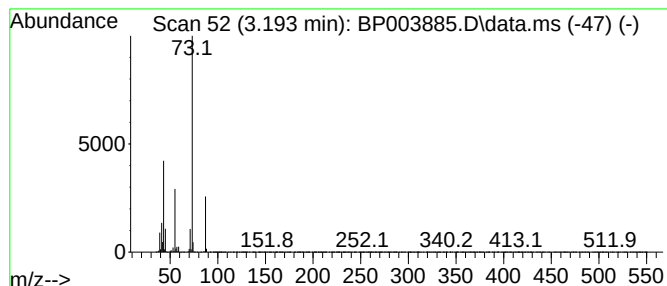
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.193	24.71 ng	1507050	1,4-Dichlorobenzene-d4	8.305

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	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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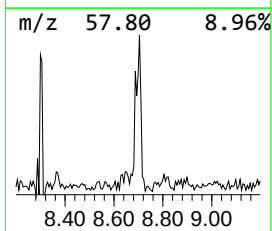
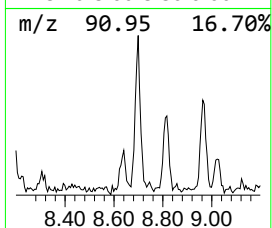
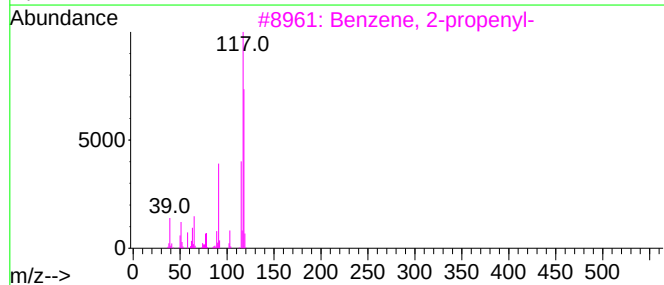
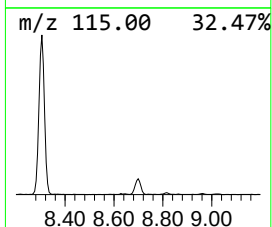
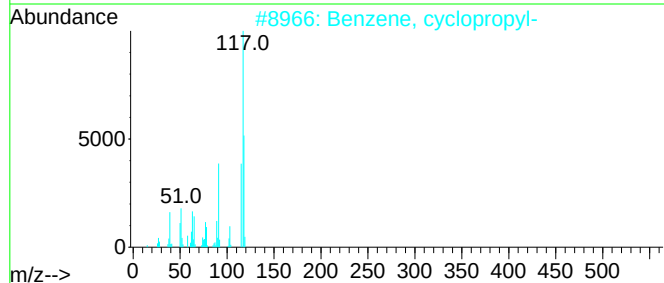
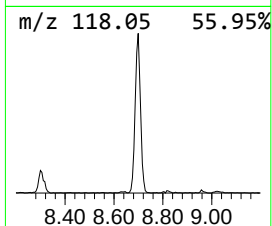
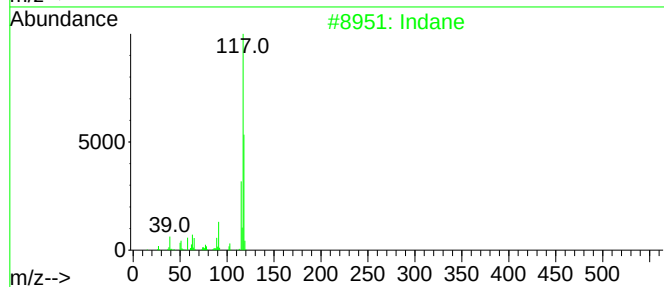
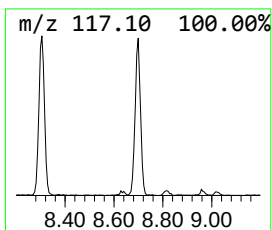
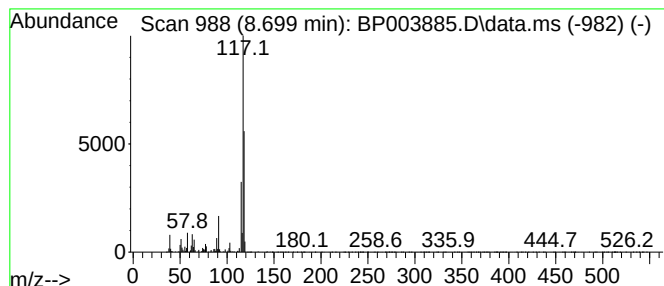
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Indane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.699	2.11 ng	128968	1,4-Dichlorobenzene-d4	8.305

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	94
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	87
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
4			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	80
5			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	74



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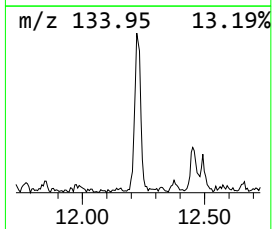
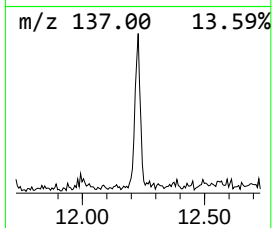
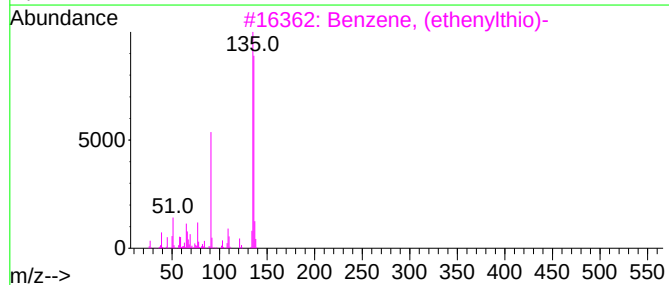
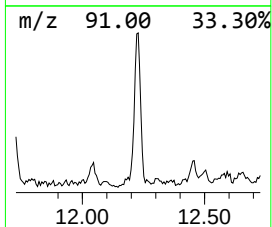
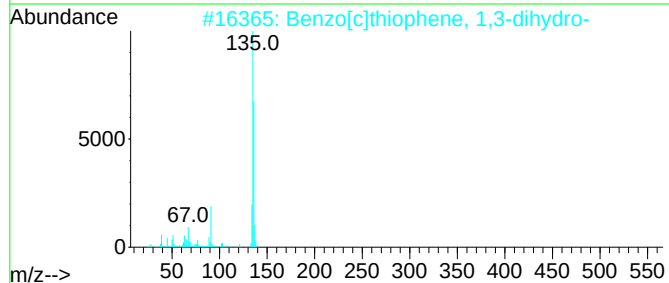
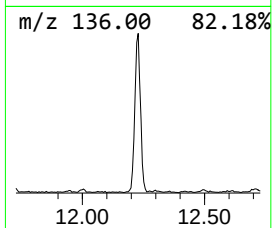
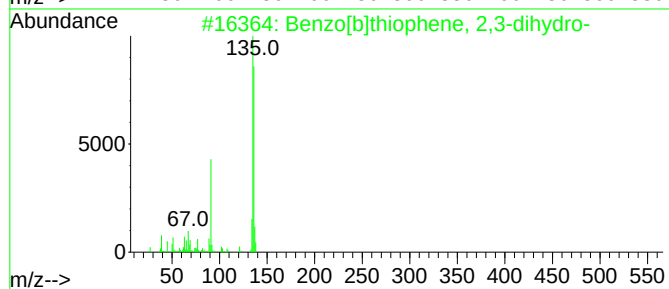
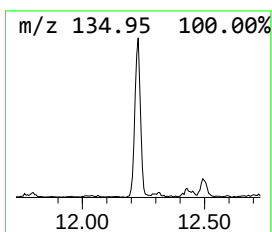
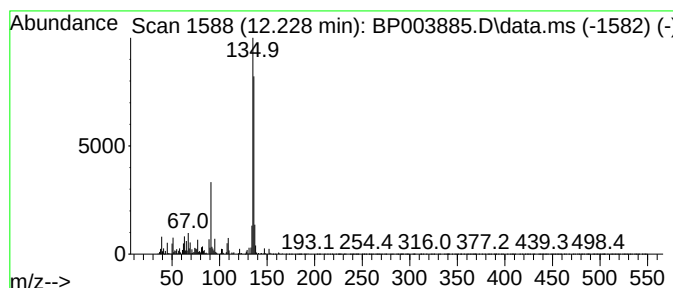
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzo[b]thiophene, 2,3-dihy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.228	2.88 ng	233954	Naphthalene-d8	11.134

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]thiophene, 2,3-dihydro-	136	C8H8S	004565-32-6	95
2			Benzo[c]thiophene, 1,3-dihydro-	136	C8H8S	002471-92-3	94
3			Benzene, (ethenylthio)-	136	C8H8S	001822-73-7	78
4			4-Hydroxy-3-methylbenzaldehyde	136	C8H8O2	015174-69-3	72
5			Benzaldehyde, 4-methoxy-	136	C8H8O2	000123-11-5	72



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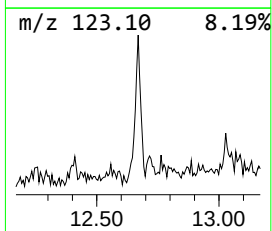
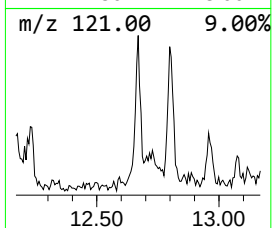
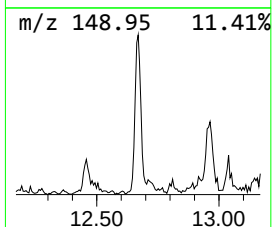
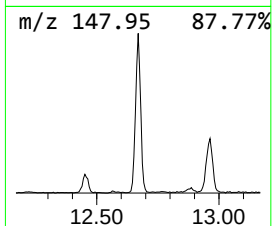
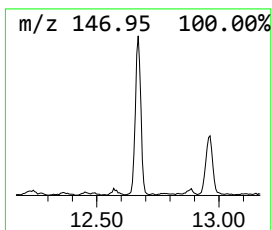
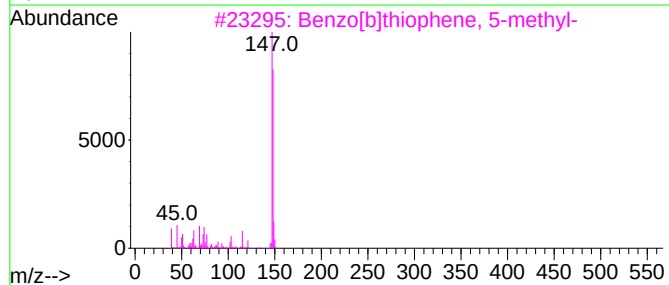
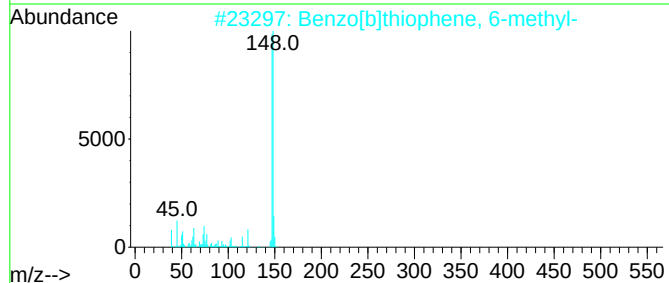
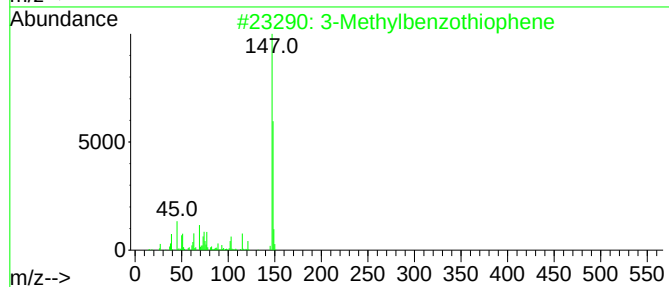
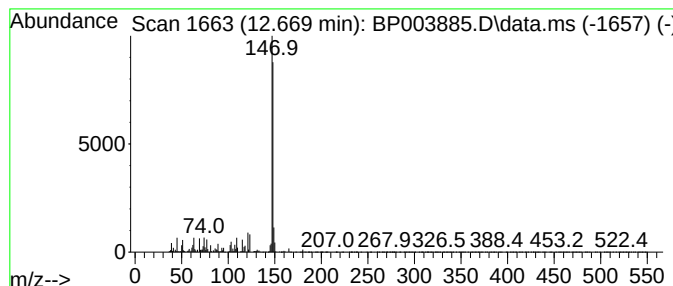
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 3-Methylbenzothiophene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.669	2.47 ng	200653	Naphthalene-d8	11.134

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Methylbenzothiophene	148	C9H8S	001455-18-1	90
2			Benzo[b]thiophene, 6-methyl-	148	C9H8S	016587-47-6	90
3			Benzo[b]thiophene, 5-methyl-	148	C9H8S	014315-14-1	90
4			Benzo[b]thiophene, 4-methyl-	148	C9H8S	014315-11-8	90
5			Benzo[b]thiophene, 2-methyl-	148	C9H8S	001195-14-8	90



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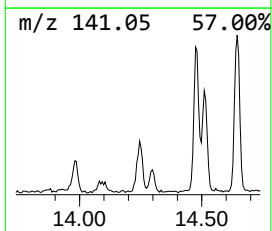
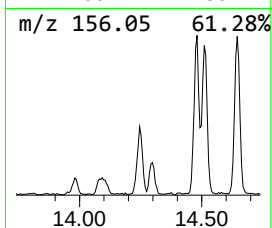
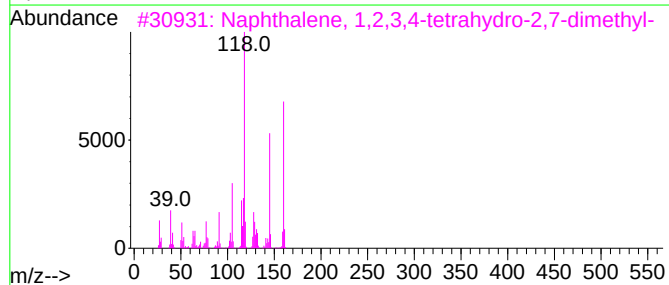
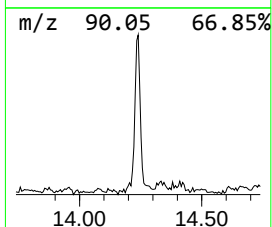
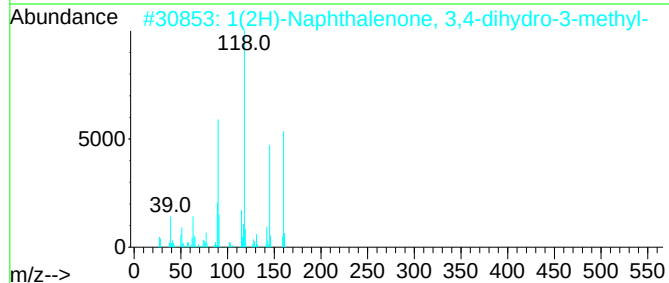
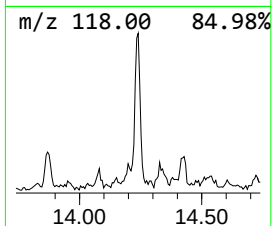
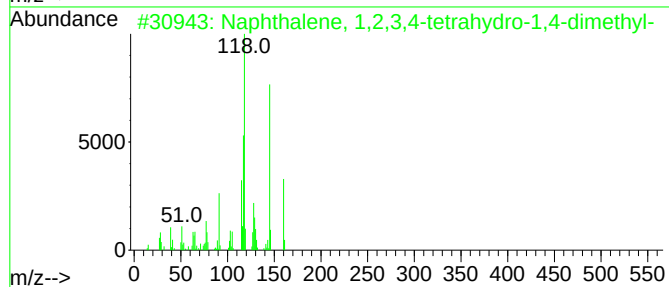
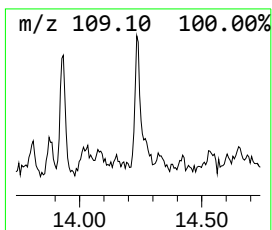
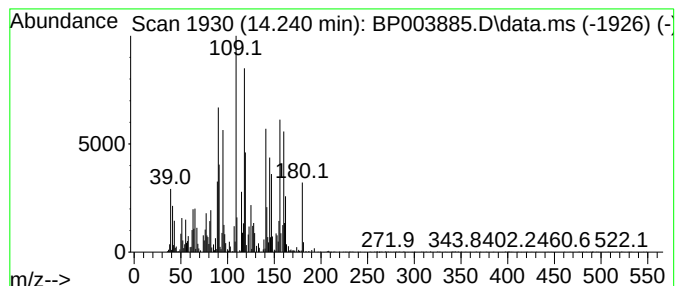
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown14.240 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.240	2.47 ng	244947	Acenaphthene-d10	14.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	38
2			1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	014944-23-1	38
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	38
4			1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	001590-08-5	30
5			4-Methylphthalic anhydride	162	C9H6O3	019438-61-0	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110920\
Data File : BP003885.D
Acq On : 10 Nov 2020 03:35
Operator : CG/JU
Sample : L4668-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-18

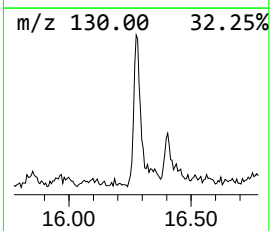
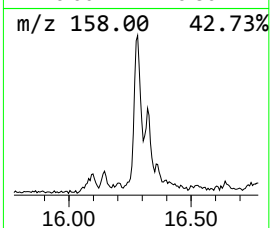
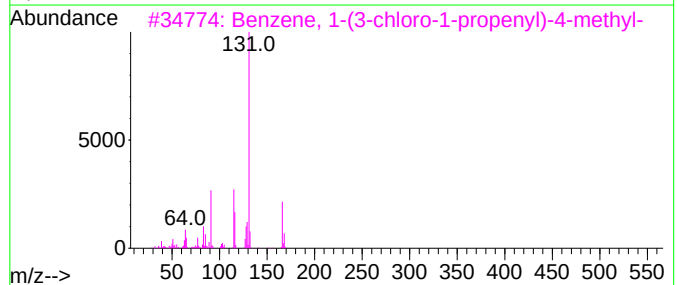
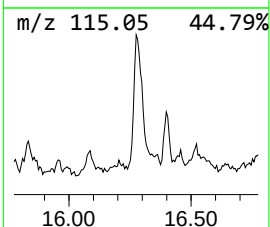
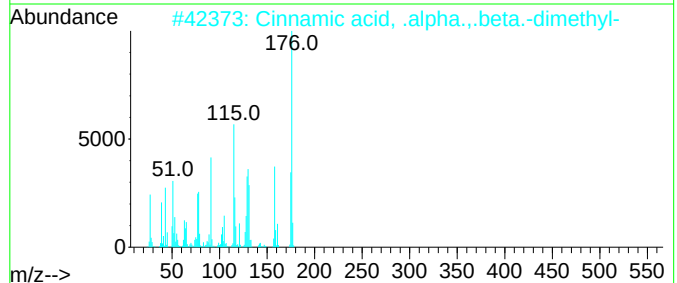
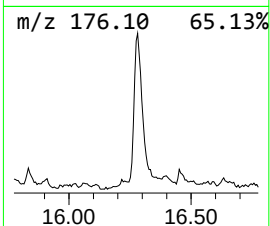
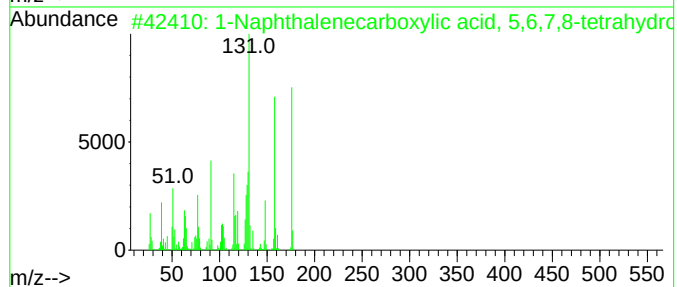
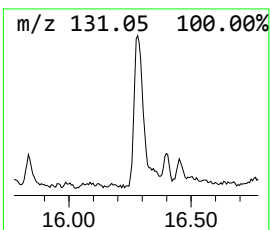
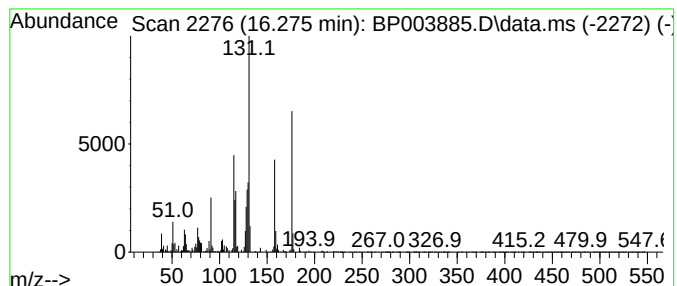
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Naphthalenecarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.275	4.07 ng	403358	Acenaphthene-d10	14.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Naphthalenecarboxylic acid, 5,...	176	C11H12O2	004242-18-6	81
2			Cinnamic acid, .alpha.,.beta.-di...	176	C11H12O2	1000151-56-4	53
3			Benzene, 1-(3-chloro-1-propenyl)...	166	C10H11Cl	1000327-36-5	38
4			3-Pentenoic acid, 4-phenyl-	176	C11H12O2	053774-19-9	38
5			Benzene, (3-chloro-1-methyl-1-pr...	166	C10H11Cl	1000327-43-7	35



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Data File : BP003885.D
Acq On : 10 Nov 2020 03:35
Operator : CG/JU
Sample : L4668-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-18

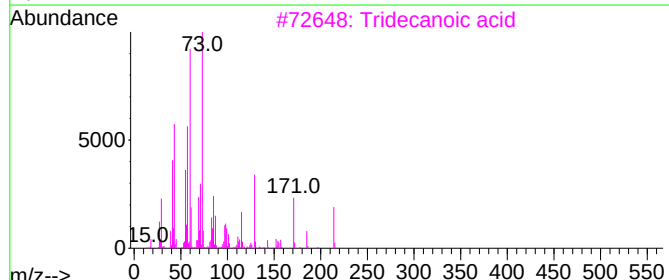
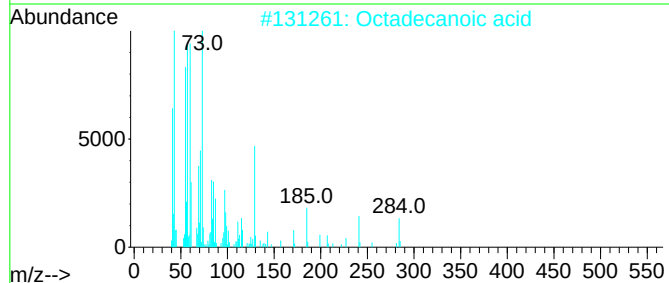
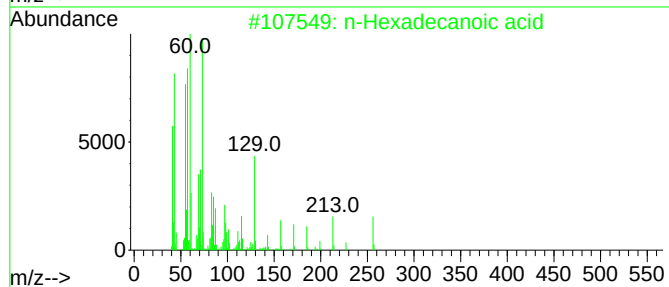
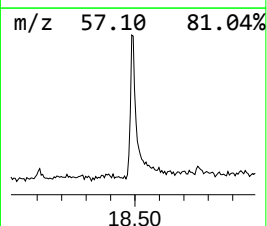
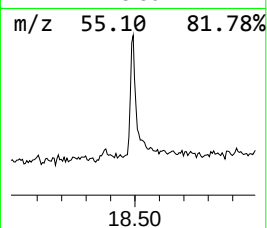
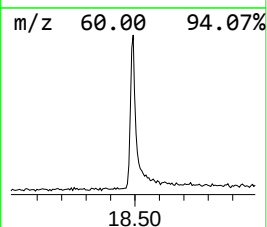
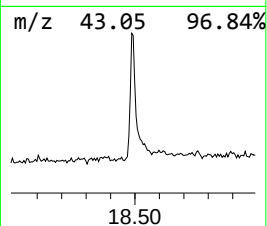
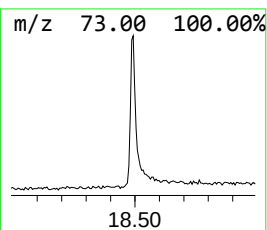
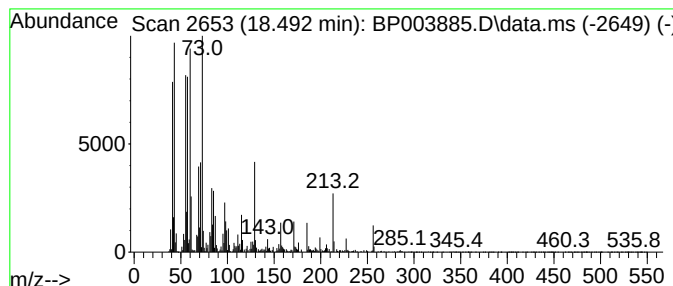
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.492	6.24 ng	582532	Phenanthrene-d10	17.651

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	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110920\
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Operator : CG/JU
Sample : L4668-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-18

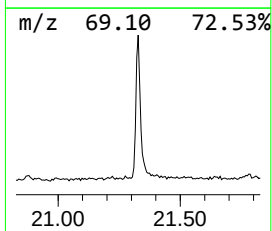
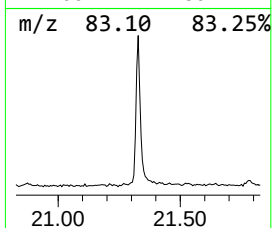
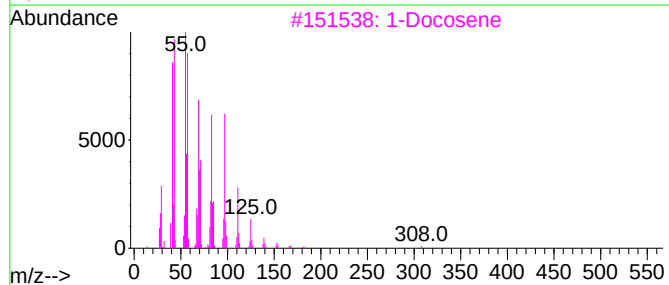
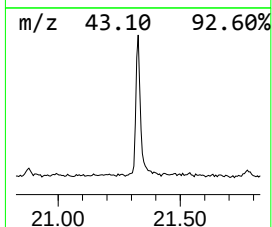
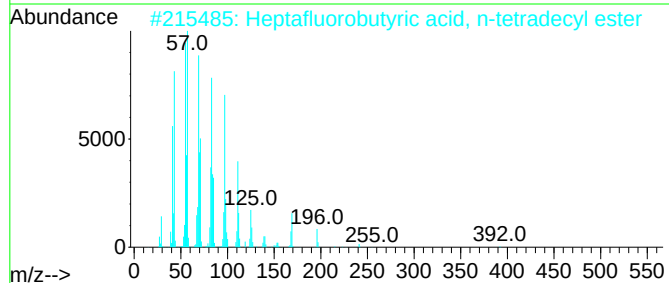
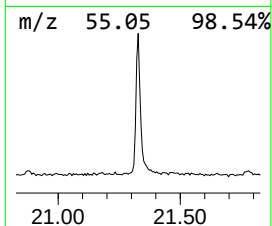
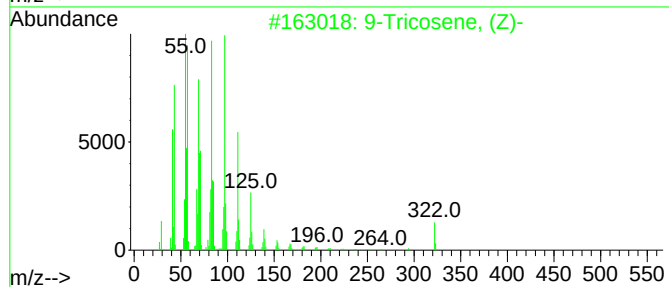
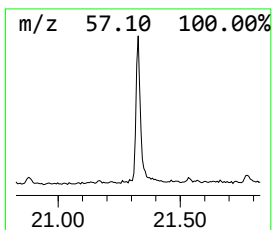
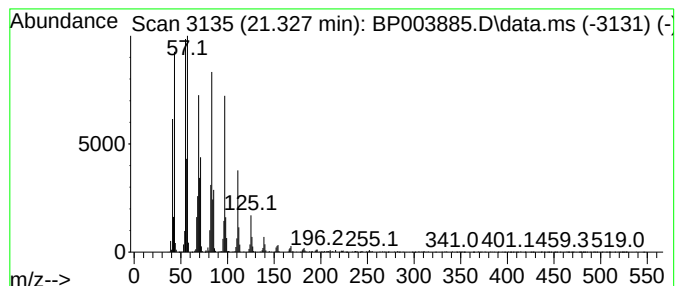
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Tricosene, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.327	13.28 ng	1138040	Chrysene-d12	21.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-			322	C23H46	027519-02-4	96
2	Heptafluorobutyric acid, n-tetra...			410	C18H29F7O2	007365-36-8	94
3	1-Docosene			308	C22H44	001599-67-3	94
4	1-Heneicosanol			312	C21H44O	015594-90-8	94
5	Trifluoroacetoxy hexadecane			338	C18H33F3O2	006222-03-3	94



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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.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...	3.193	24.7	ng	1507050	1	8.305	1219960	20.0
Indane	8.699	2.1	ng	128968	1	8.305	1219960	20.0
Benzo[b]thiophe...	12.228	2.9	ng	233954	2	11.134	1623450	20.0
3-Methylbenzoth...	12.669	2.5	ng	200653	2	11.134	1623450	20.0
unknown14.240	14.240	2.5	ng	244947	3	14.922	1983110	20.0
1-Naphthaleneca...	16.275	4.1	ng	403358	3	14.922	1983110	20.0
n-Hexadecanoic ...	18.492	6.2	ng	582532	4	17.651	1866720	20.0
9-Tricosene, (Z)-	21.327	13.3	ng	1138040	5	21.674	1714500	20.0