LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100422\
Data File : BF130522.D
Acq On : 04 Oct 2022 17:14
Operator : CG\JU
Sample : N4941-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-6R

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-BF091422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130522.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.128	343	347	354	rBV	143397	184400	7.42%	1.338%
2	4.804	457	462	480	rBV	718909	868345	34.95%	6.301%
3	5.234	532	535	546	rBV	664973	672071	27.05%	4.877%
4	5.640	600	604	614	rBV	171021	164022	6.60%	1.190%
5	6.269	708	711	722	rBV	422708	465615	18.74%	3.379%
6	6.628	769	772	776	rBV	516462	462688	18.62%	3.358%
7	6.810	798	803	808	rBV	71971	62665	2.52%	0.455%
8	7.198	865	869	872	rBV	1590306	1430664	57.58%	10.382%
9	7.339	887	893	896	rBV	22348	32614	1.31%	0.237%
10	7.910	987	990	993	rBV	644795	616820	24.83%	4.476%
11	7.933	993	994	997	rVB	227044	134639	5.42%	0.977%
12	8.722	1123	1128	1132	rVB2	32794	32960	1.33%	0.239%
13	8.992	1169	1174	1177	rBV	3162439	2484660	100.00%	18.031%
14	9.439	1247	1250	1255	rBV	32978	36023	1.45%	0.261%
15	9.522	1261	1264	1269	rBV	42521	37938	1.53%	0.275%
16	9.663	1284	1288	1291	rBV	736753	579120	23.31%	4.203%
17	9.692	1291	1293	1297	rVB	620885	512310	20.62%	3.718%
18	9.822	1309	1315	1317	rBV2	34632	32799	1.32%	0.238%
19	9.869	1317	1323	1326	rBV	182200	157026	6.32%	1.139%
20	10.210	1377	1381	1385	rVB2	36197	36528	1.47%	0.265%
21	10.275	1387	1392	1393	rBV	33262	38308	1.54%	0.278%
22	10.369	1405	1408	1412	rVB	36139	35311	1.42%	0.256%
23	10.451	1418	1422	1428	rBV	991246	893946	35.98%	6.487%
24	10.639	1451	1454	1458	rBV2	30108	35137	1.41%	0.255%
25	11.145	1536	1540	1543	rBV	546798	482344	19.41%	3.500%
26	11.686	1628	1632	1635	rBV2	54464	60134	2.42%	0.436%
27	12.351	1742	1745	1750	rBV	52081	44193	1.78%	0.321%
28	12.580	1778	1784	1787	rBV	29099	34920	1.41%	0.253%
29	12.727	1805	1809	1813	rBV	1815465	1658660	66.76%	12.036%
30	13.774	1980	1987	1999	rBV	487317	481504	19.38%	3.494%
31	14.533	2112	2116	2124	rBV	284284	290607	11.70%	2.109%
32	15.162	2218	2223	2232	rBV	424748	499070	20.09%	3.622%
33	18.827	2835	2846	2855	rBV3	68611	222262	8.95%	1.613%

Sum of corrected areas: 13780303

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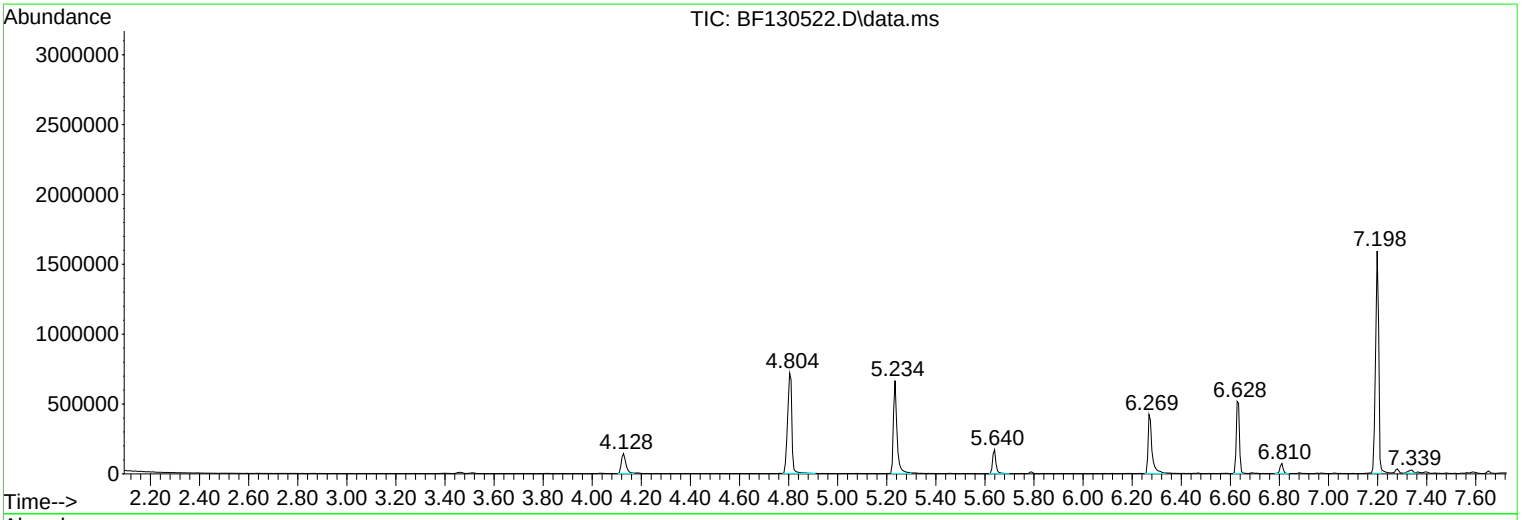
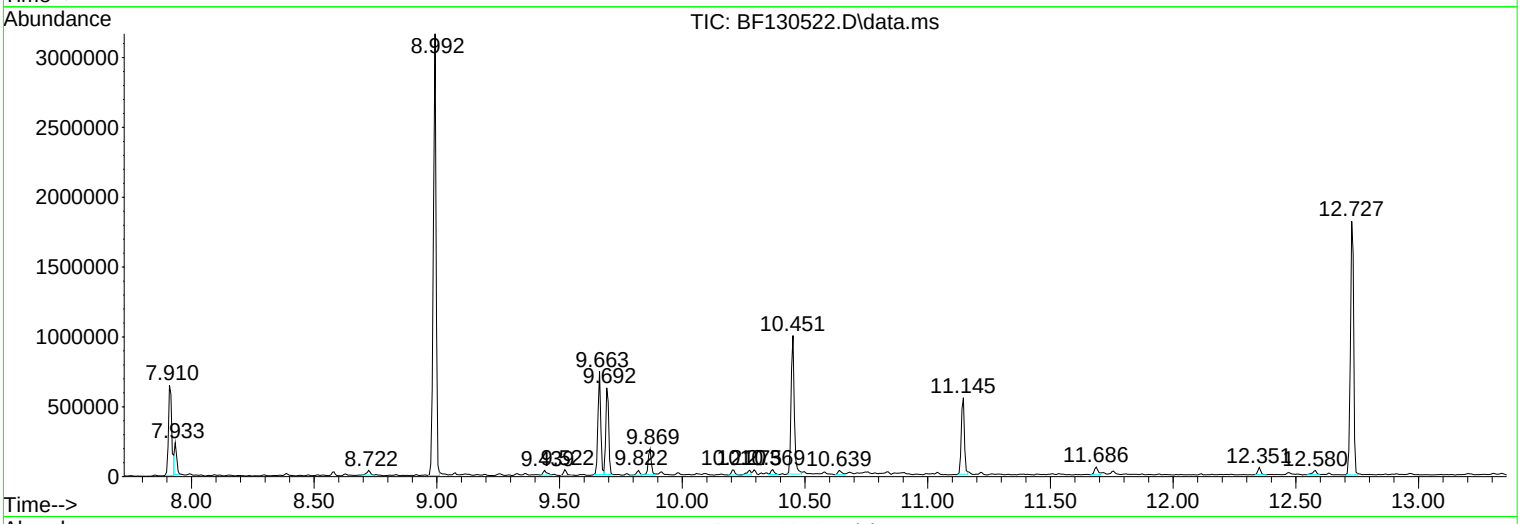
Misc :
ALS Vial : 12 Sample Multiplier: 1

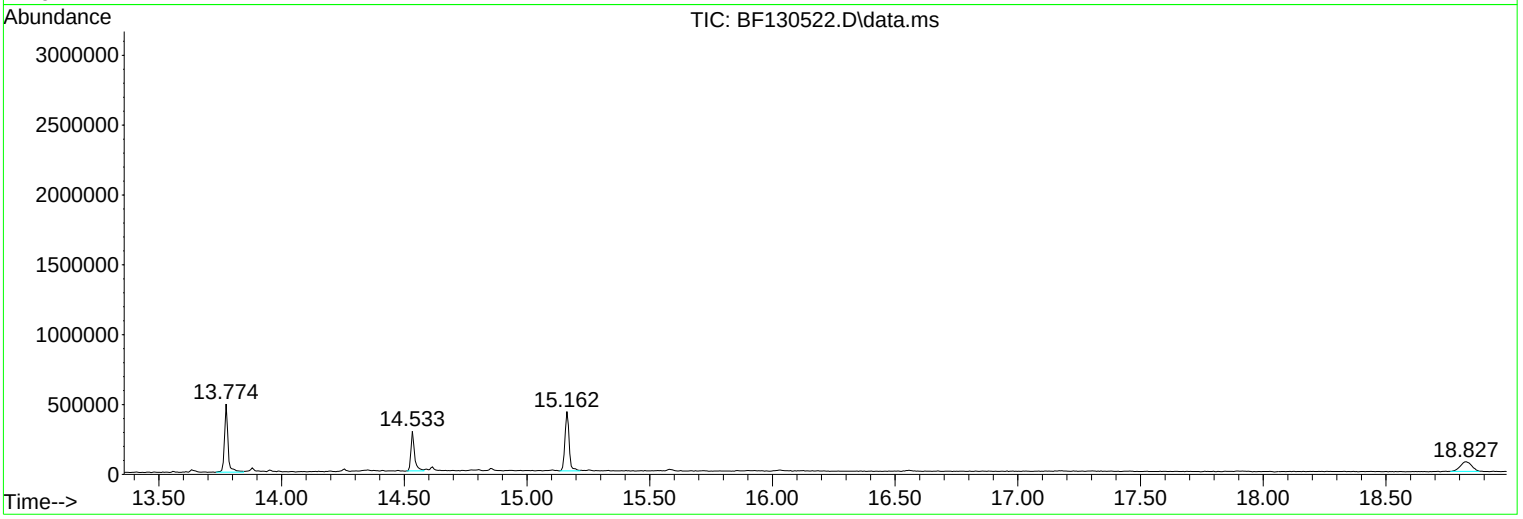
Instrument :
BNA_F
ClientSampleId :
MW-6R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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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Data File : BF130522.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

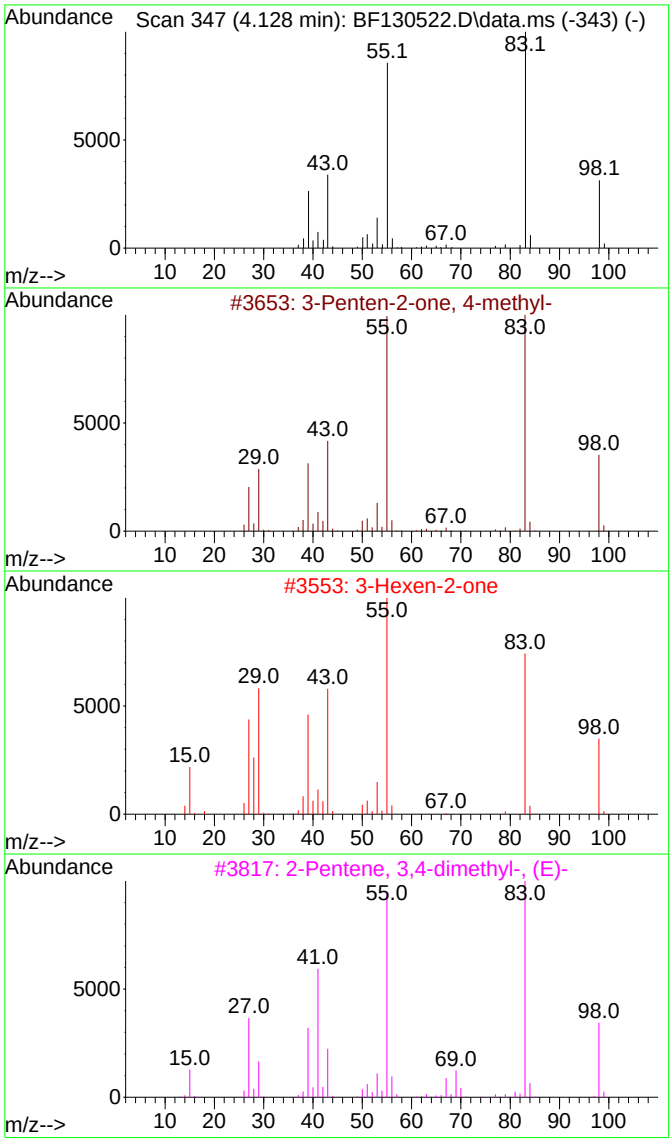
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

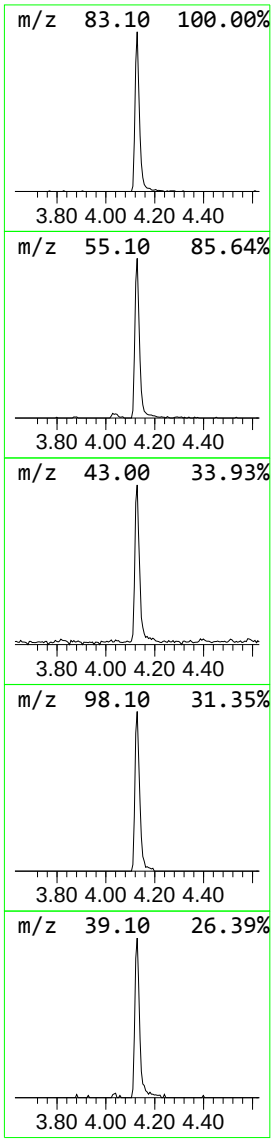
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.128	7.97 ng	184400	1,4-Dichlorobenzene-d4	6.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





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Instrument :
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ClientSampleId :
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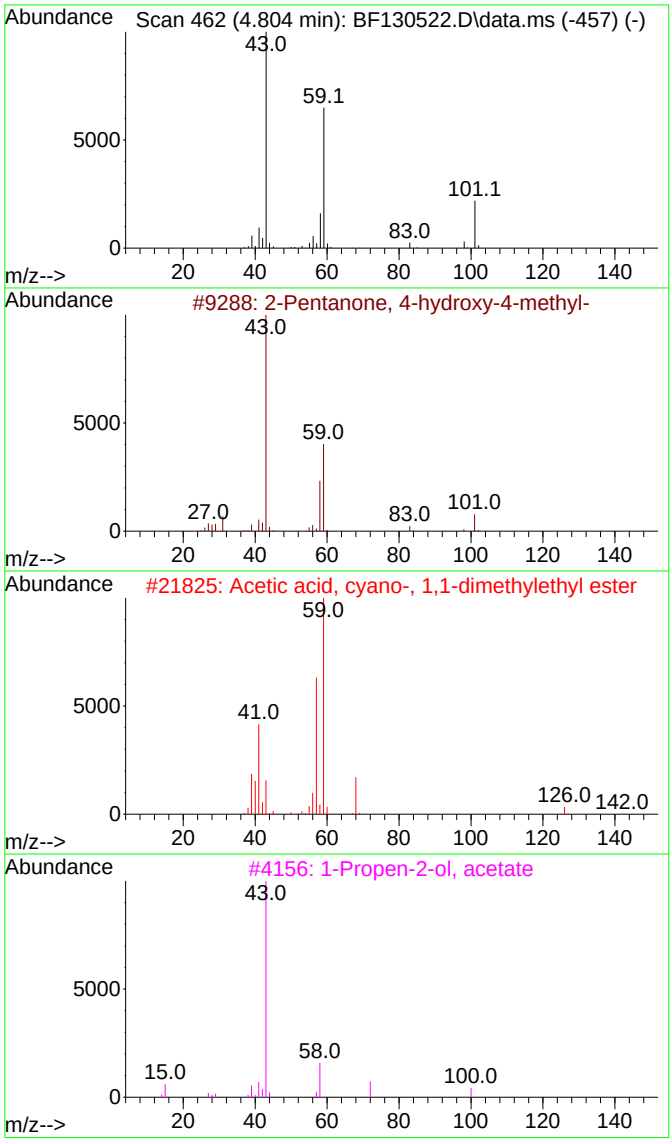
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

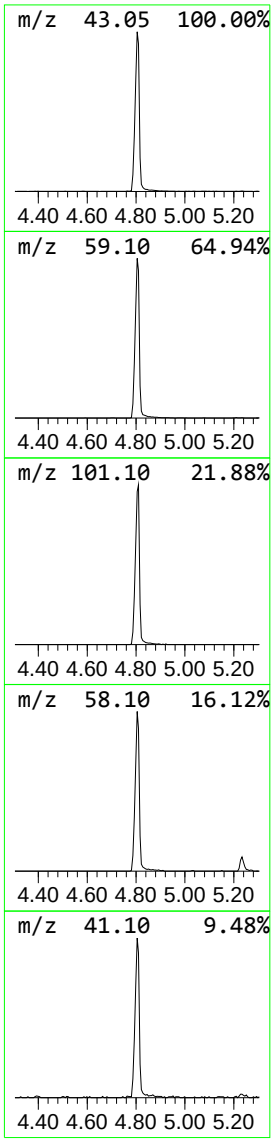
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.804	37.53 ng	868345	1,4-Dichlorobenzene-d4	6.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Operator : CG\JU
Sample : N4941-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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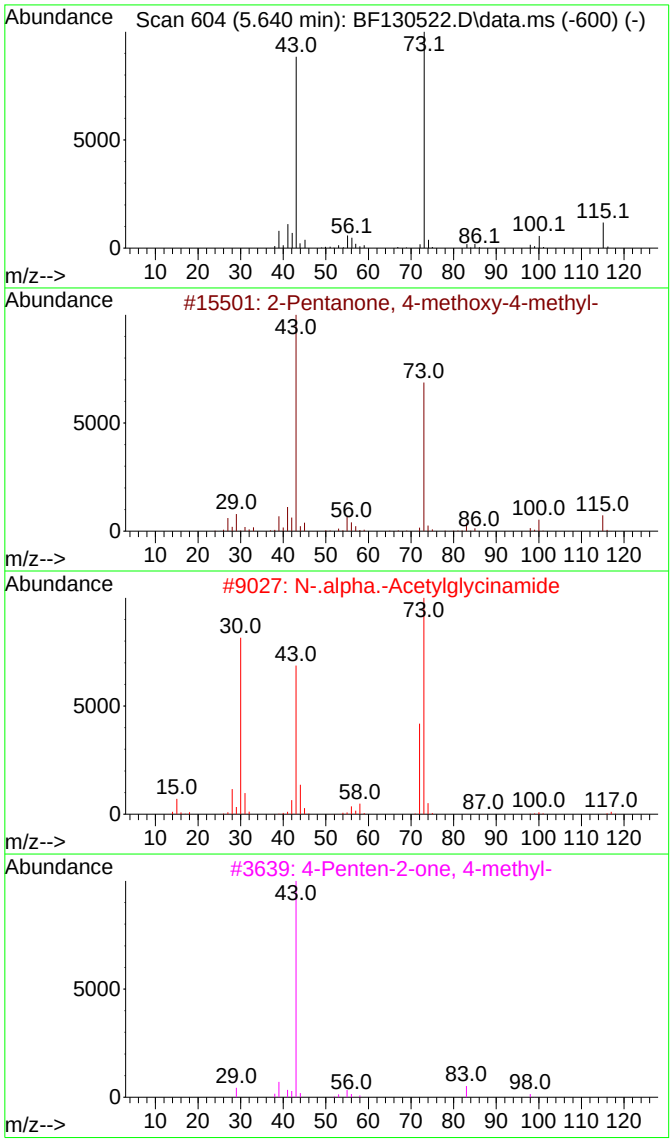
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

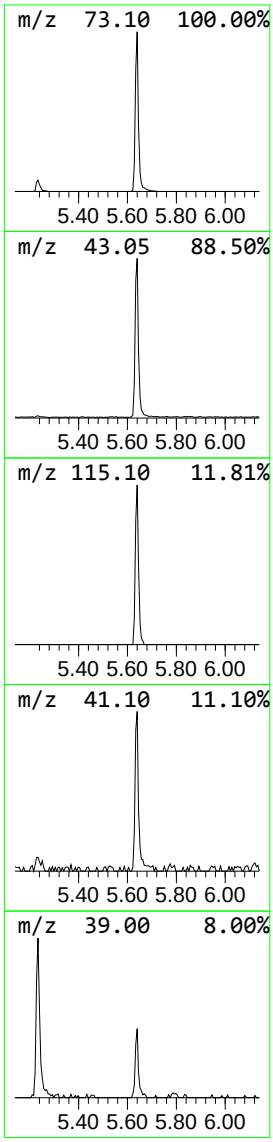
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.640	7.09 ng	164022	1,4-Dichlorobenzene-d4	6.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	47
3	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	10
4	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
5	Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9





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Sample : N4941-02
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
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TIC Library : C:\Database\NIST20.L
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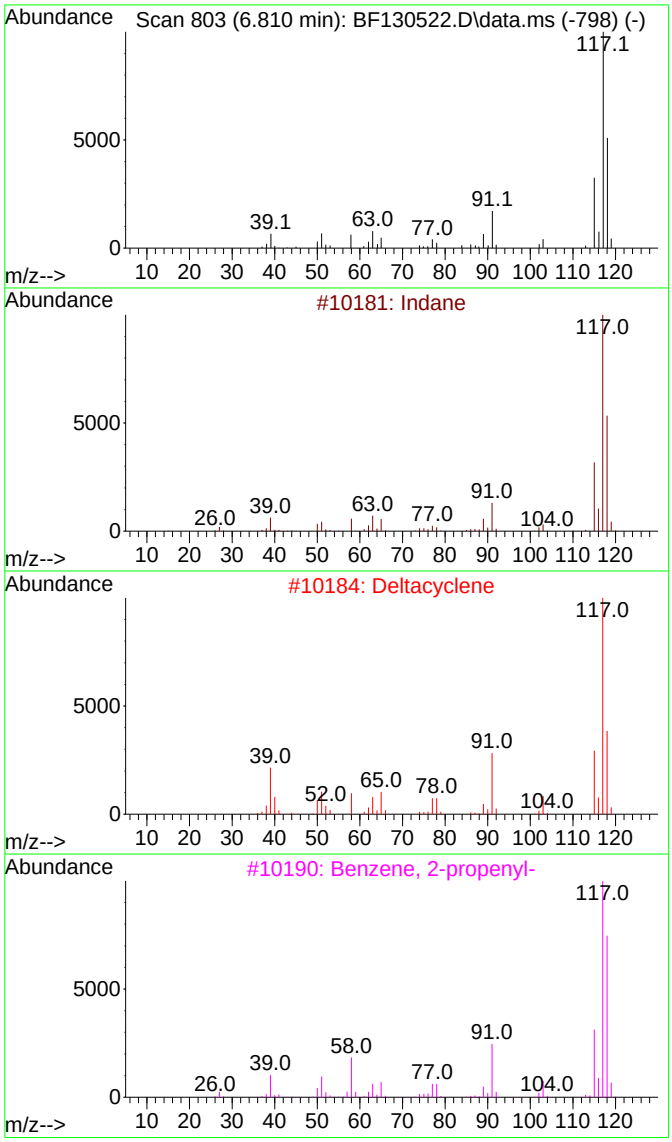
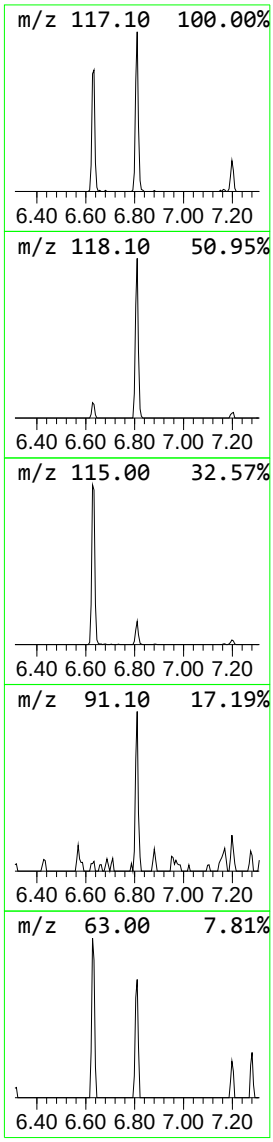
****

Peak Number 4 Indane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.810	2.71 ng	62665	1,4-Dichlorobenzene-d4	6.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Deltacyclene	118	C9H10	007785-10-6	81
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
5	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	60





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

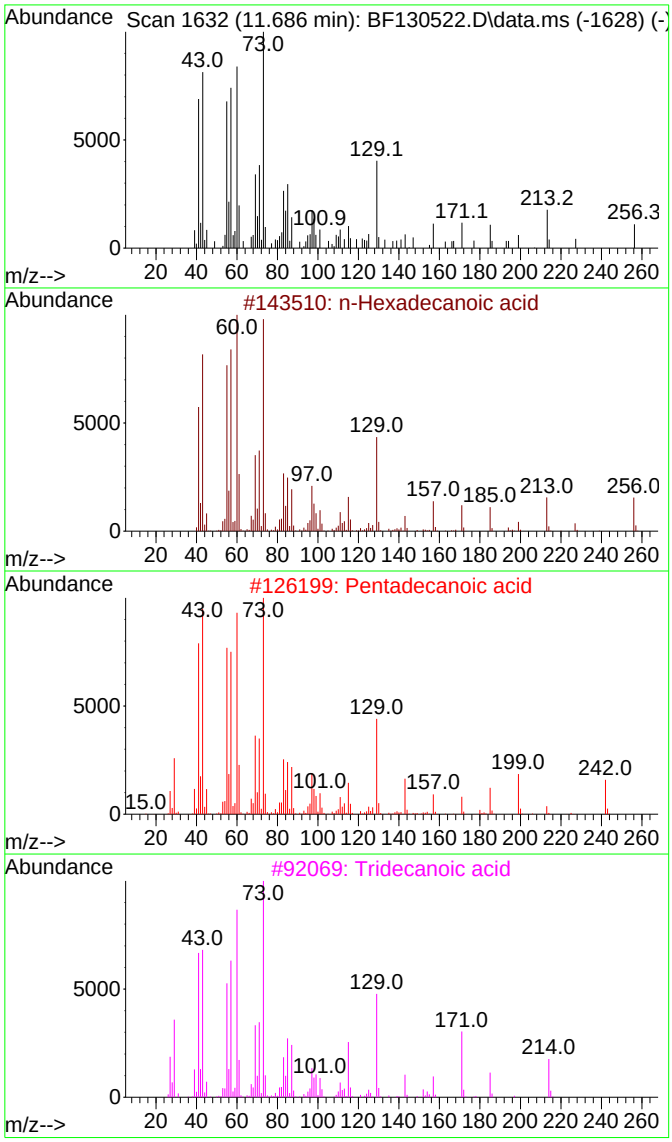
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

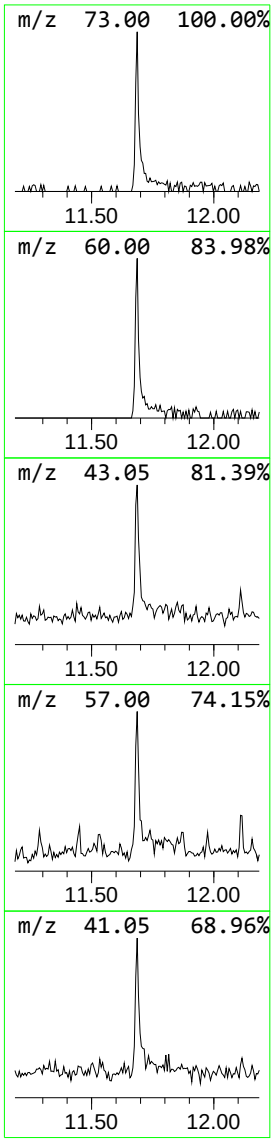
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.686	2.49 ng	60134	Phenanthrene-d10	11.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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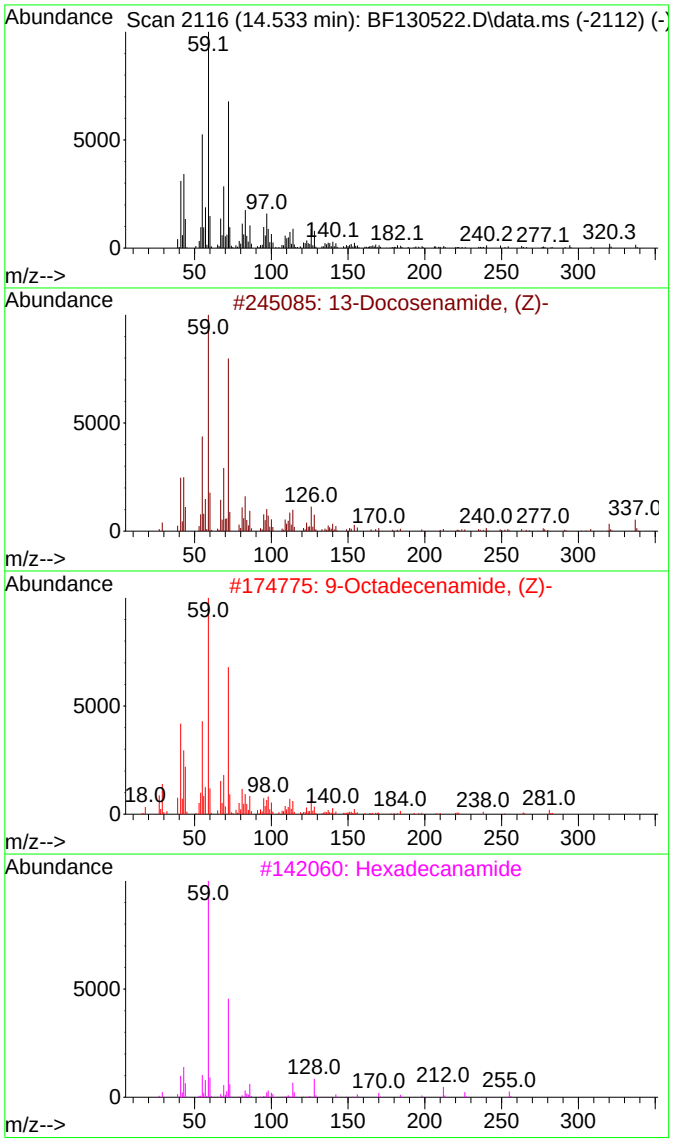
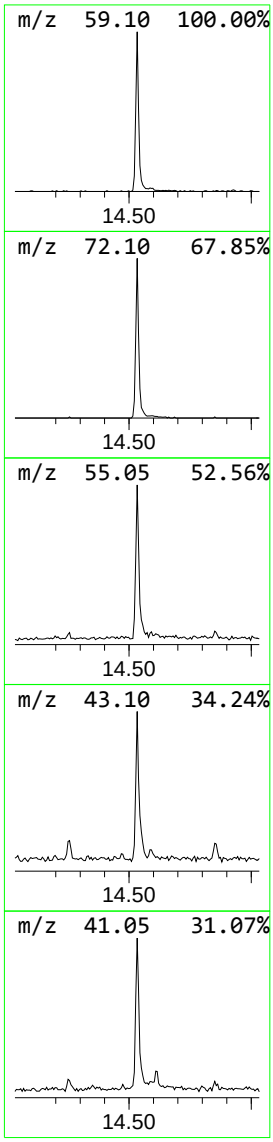
****

Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.533	11.65 ng	290607	Perylene-d12	15.162

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	96
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3	Hexadecanamide	255	C16H33NO	000629-54-9	72
4	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	64
5	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	59





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Instrument :
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ClientSampleId :
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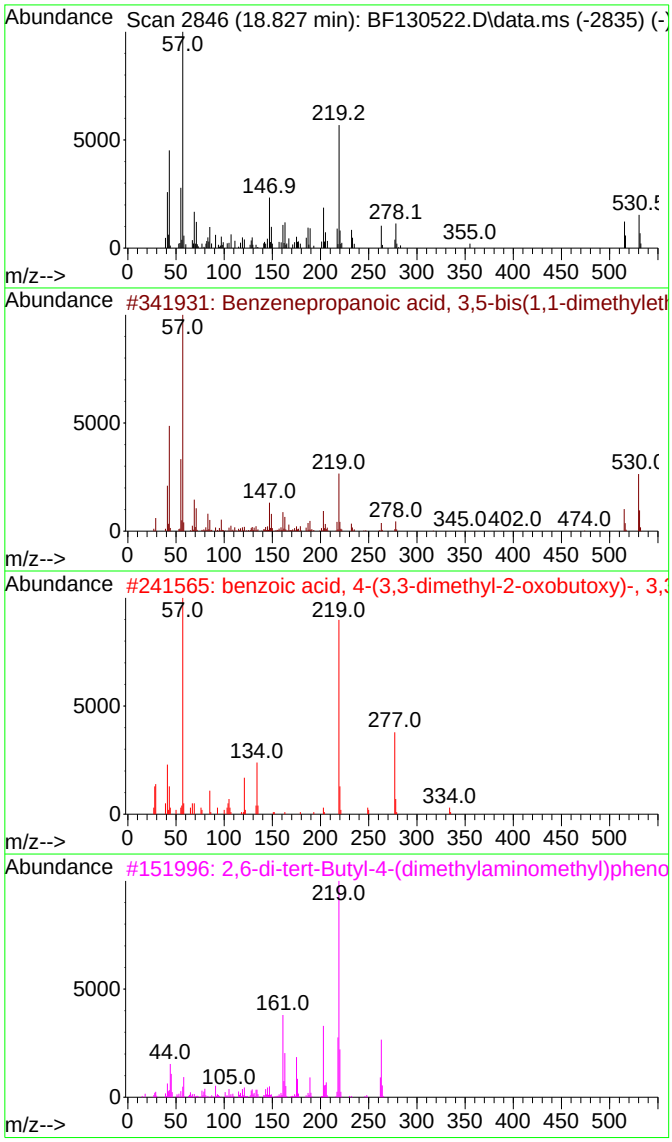
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

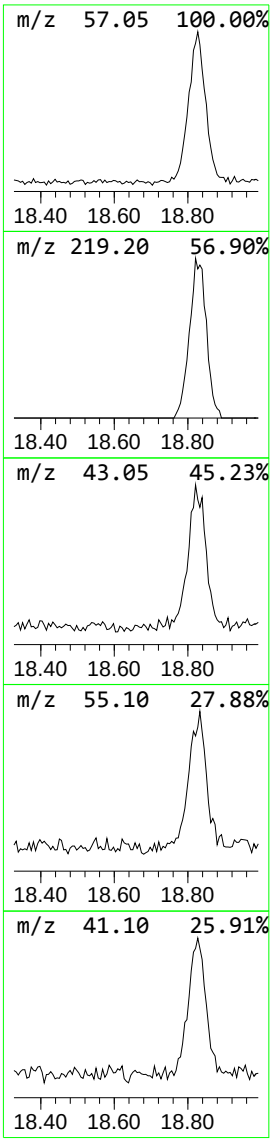
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzenepropanoic acid, 3,5-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.827	8.91 ng	222262	Perylene-d12	15.162

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenepropanoic acid, 3,5-bis(1...	530	C35H62O3	002082-79-3	96
2	benzoic acid, 4-(3,3-dimethyl-2-...	334	C19H26O5	1010398-08-2	27
3	2,6-di-tert-Butyl-4-(dimethylami...	263	C17H29NO	000088-27-7	25
4	2H-1-benzopyran-3-carboxylic aci...	278	C15H18O5	1000397-12-1	25
5	Chromone, 5-hydroxy-8-isopentyl-...	276	C16H20O4	013475-10-0	22





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one,...	4.128	8.0	ng	184400	1	6.634	462688	20.0
2-Pentanone, 4-...	4.804	37.5	ng	868345	1	6.634	462688	20.0
2-Pentanone, 4-...	5.640	7.1	ng	164022	1	6.634	462688	20.0
Indane	6.810	2.7	ng	62665	1	6.634	462688	20.0
n-Hexadecanoic ...	11.686	2.5	ng	60134	4	11.145	482344	20.0
13-Docosenamide...	14.533	11.7	ng	290607	6	15.162	499070	20.0
Benzenepropanoi...	18.827	8.9	ng	222262	6	15.162	499070	20.0