LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131017.D
Acq On : 05 Nov 2022 13:42
Operator : CG\JU
Sample : N5340-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-8-102722

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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131017.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	10	18	23	rVB	1256769	1640023	64.06%	10.590%
2	2.310	33	38	45	rVB	21155	31439	1.23%	0.203%
3	5.122	512	516	522	rBV	153084	170516	6.66%	1.101%
4	5.516	579	583	587	rBV	1158532	1072296	41.88%	6.924%
5	6.157	687	692	696	rBV	39271	35298	1.38%	0.228%
6	6.522	750	754	766	rVB	762970	718049	28.05%	4.637%
7	6.904	815	819	822	rBV	446032	381822	14.91%	2.466%
8	7.304	883	887	890	rBV2	22342	26515	1.04%	0.171%
9	7.469	909	915	918	rBV	1576576	1565908	61.16%	10.112%
10	7.510	918	922	925	rVV2	68106	63531	2.48%	0.410%
11	7.581	931	934	937	rVB	81914	66457	2.60%	0.429%
12	7.710	949	956	962	rBV	122307	202167	7.90%	1.305%
13	7.787	965	969	971	rBV2	36541	34901	1.36%	0.225%
14	7.898	984	988	991	rBV	59044	62309	2.43%	0.402%
15	7.934	991	994	998	rVV2	41002	41154	1.61%	0.266%
16	7.992	999	1004	1008	rVB4	24767	25979	1.01%	0.168%
17	8.110	1016	1024	1029	rBV4	25464	60480	2.36%	0.391%
18	8.187	1033	1037	1040	rVB	609200	491559	19.20%	3.174%
19	8.551	1094	1099	1103	rBV5	26073	49280	1.92%	0.318%
20	8.786	1135	1139	1142	rVB2	54403	72509	2.83%	0.468%
21	8.916	1158	1161	1164	rBV2	46823	51755	2.02%	0.334%
22	9.269	1215	1221	1224	rBV	2574251	2560239	100.00%	16.532%
23	9.375	1234	1239	1246	rVB2	178512	287126	11.21%	1.854%
24	9.481	1254	1257	1262	rVB	29531	35435	1.38%	0.229%
25	9.698	1291	1294	1299	rVB6	31671	39228	1.53%	0.253%
26	9.757	1299	1304	1307	rVB3	44256	43804	1.71%	0.283%
27	9.863	1317	1322	1326	rVB3	84321	119844	4.68%	0.774%
28	9.945	1332	1336	1340	rBV	637042	551397	21.54%	3.561%
29	10.086	1357	1360	1365	rVB4	29146	36966	1.44%	0.239%
30	10.139	1365	1369	1370	rBV4	20585	26468	1.03%	0.171%
31	10.263	1388	1390	1393	rBV	41001	37931	1.48%	0.245%
32	10.739	1466	1471	1478	rBV	1556045	1447205	56.53%	9.345%
33	10.845	1487	1489	1493	rVB	35254	26375	1.03%	0.170%
34	11.304	1564	1567	1575	rVB6	22725	38924	1.52%	0.251%
35	11.439	1587	1590	1594	rVB	643563	487682	19.05%	3.149%
36	11.822	1653	1655	1658	rVB2	43835	33062	1.29%	0.213%

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Misc :
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Instrument :
BNA_F
ClientSampleId :
MW-8-102722

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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.963	1674	1679	1682	rBV	53973	65111	2.54%	0.420%
38	12.580	1781	1784	1787	rVB2	30800	26299	1.03%	0.170%
39	12.745	1808	1812	1818	rVB5	18097	30096	1.18%	0.194%
40	13.033	1856	1861	1864	rBV	2081675	1868053	72.96%	12.063%
41	13.974	2018	2021	2026	rVB6	20878	29151	1.14%	0.188%
42	14.086	2037	2040	2043	rVB	418456	344976	13.47%	2.228%
43	14.198	2056	2059	2062	rVB	69238	61103	2.39%	0.395%
44	15.592	2291	2296	2304	rBV	321206	425689	16.63%	2.749%

Sum of corrected areas: 15486111

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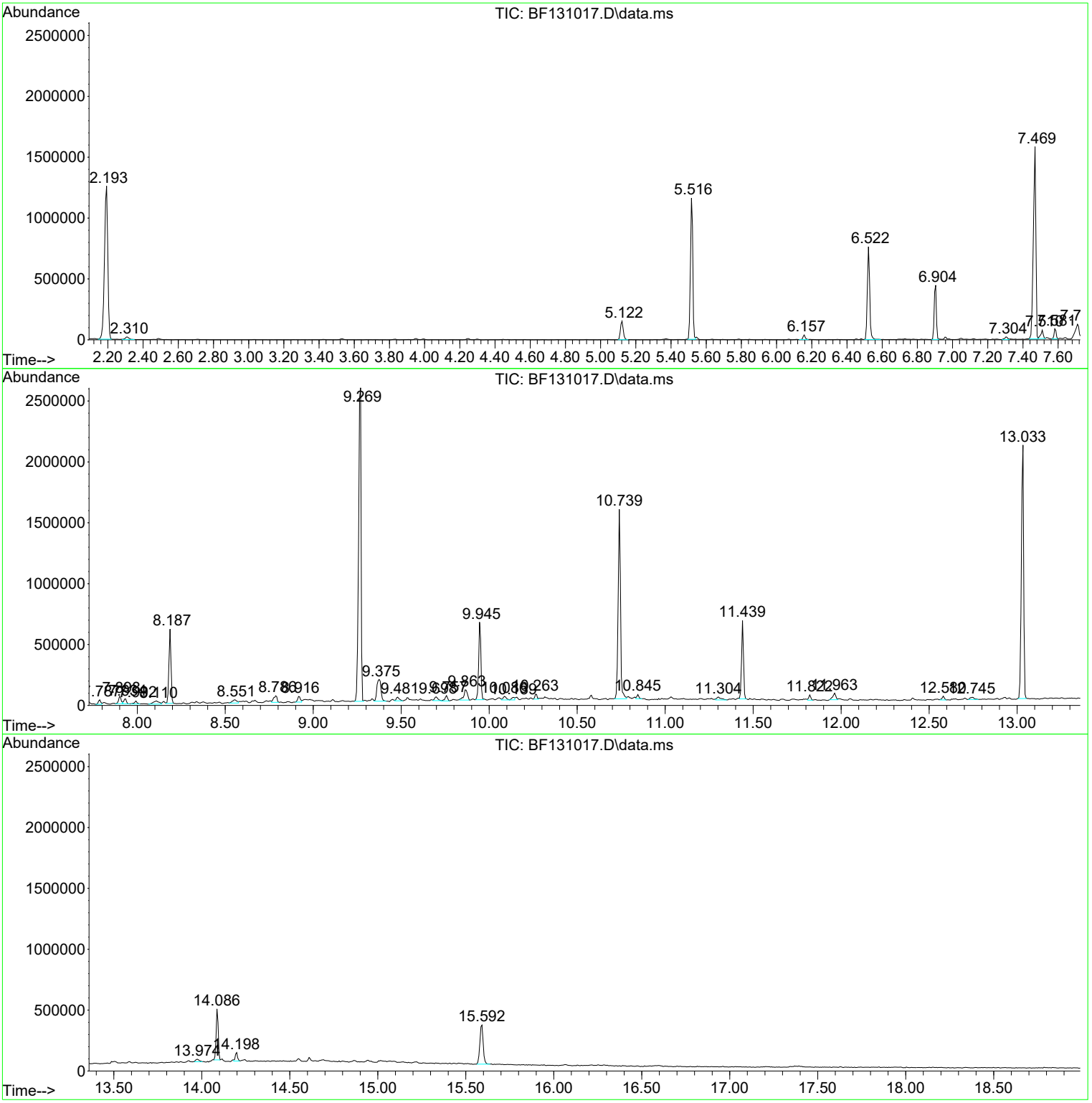
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131017.D
Acq On : 05 Nov 2022 13:42
Operator : CG\JU
Sample : N5340-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-8-102722

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

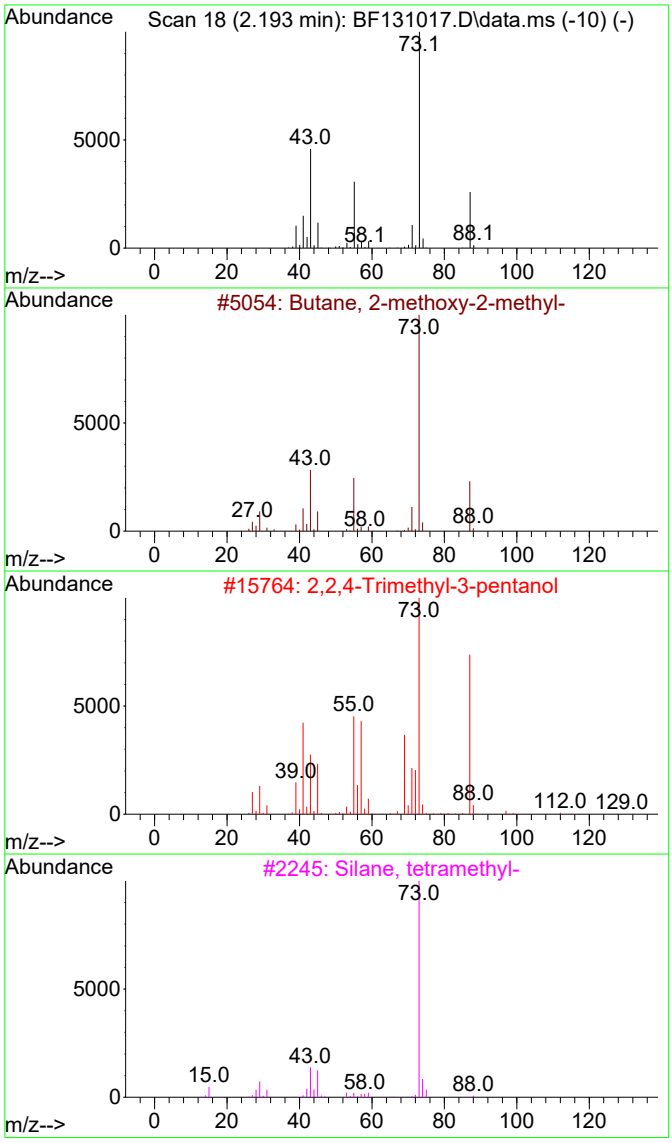
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

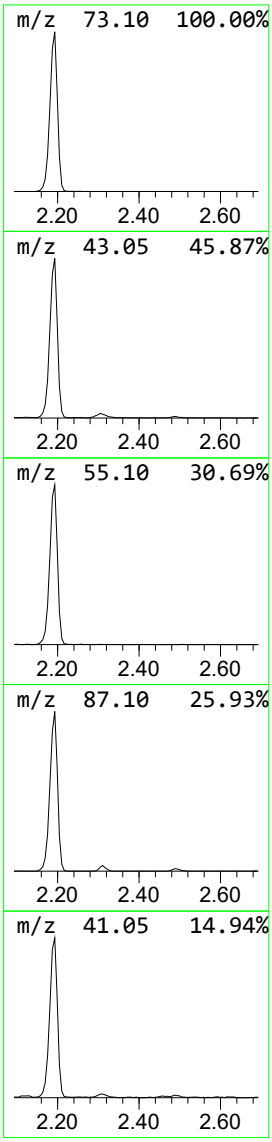
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	85.91 ng	1640020	1,4-Dichlorobenzene-d4	6.904

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Sample : N5340-04
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ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-8-102722

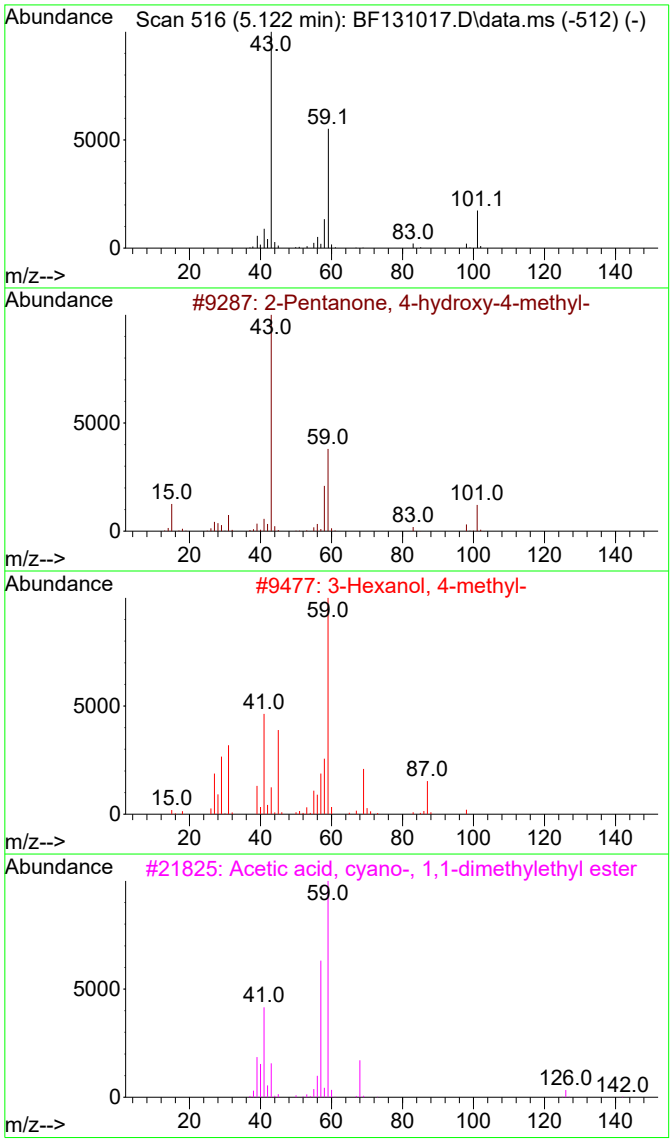
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

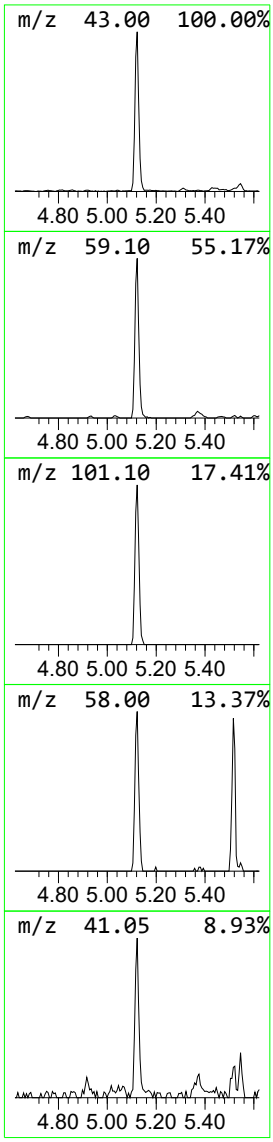
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	8.93 ng	170516	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Acq On : 05 Nov 2022 13:42
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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

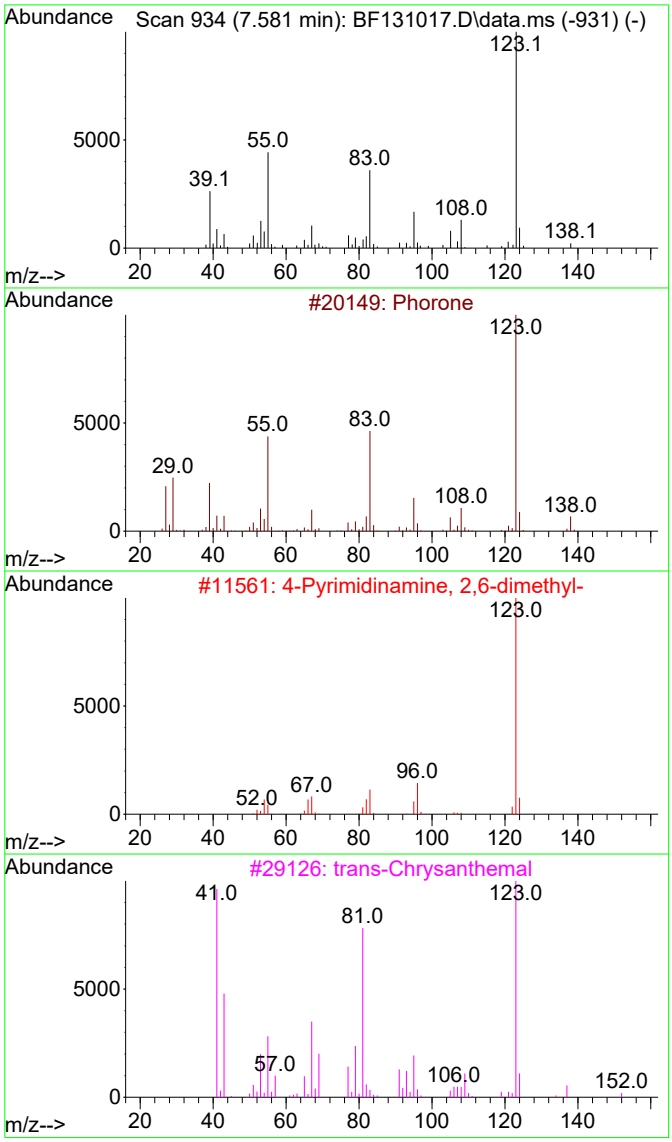
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

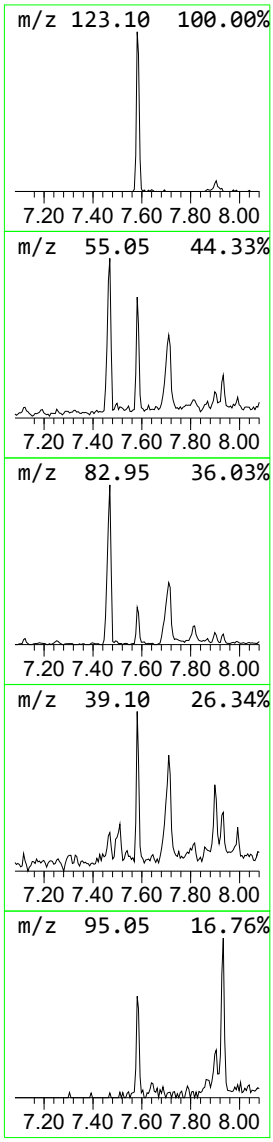
****

Peak Number 3 Phorone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.581	2.70 ng	66457	Naphthalene-d8	8.187

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phorone	138	C9H14O	000504-20-1	83
2	4-Pyrimidinamine, 2,6-dimethyl-	123	C6H9N3	000461-98-3	59
3	trans-Chrysanthemal	152	C10H16O	020104-05-6	53
4	2-Pyrimidinamine, 4,6-dimethyl-	123	C6H9N3	000767-15-7	53
5	4-Fluorobenzoic acid, undec-2-en...	292	C18H25FO2	1000299-15-8	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131017.D
Acq On : 05 Nov 2022 13:42
Operator : CG\JU
Sample : N5340-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-8-102722

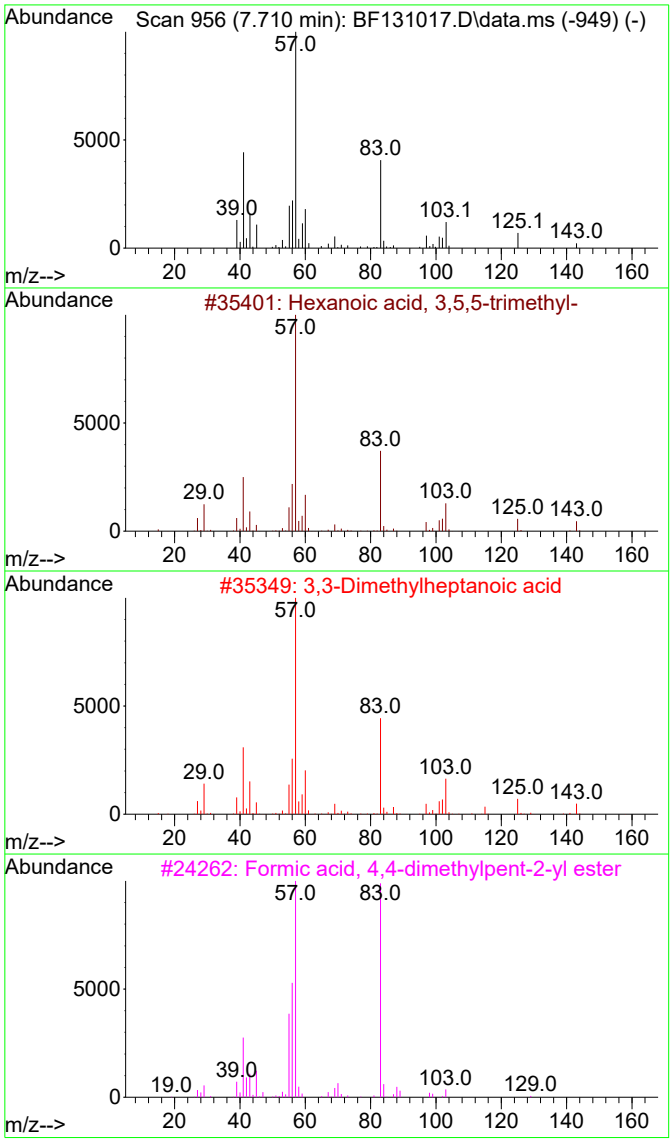
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

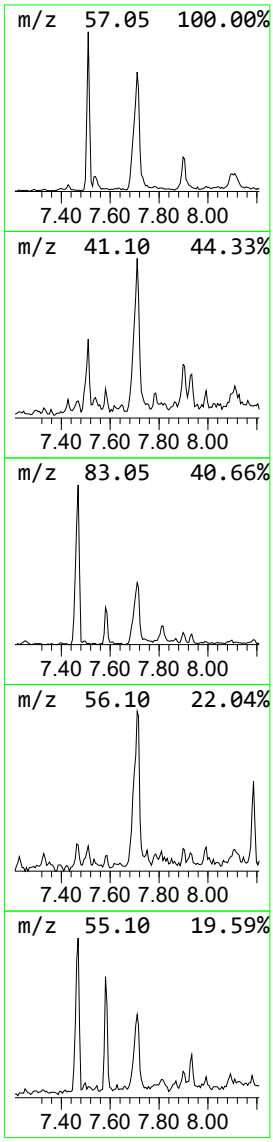
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Hexanoic acid, 3,5,5-trimet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.710	8.23 ng	202167	Naphthalene-d8	8.187

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	90
2	3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	83
3	Formic acid, 4,4-dimethylpent-2-...	144	C8H16O2	1000368-69-9	43
4	Hexanoyl chloride, 3,5,5-trimethyl-	176	C9H17ClO	036727-29-4	42
5	6,6-Dimethylheptanoic acid	158	C9H18O2	015898-92-7	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131017.D
Acq On : 05 Nov 2022 13:42
Operator : CG\JU
Sample : N5340-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-8-102722

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

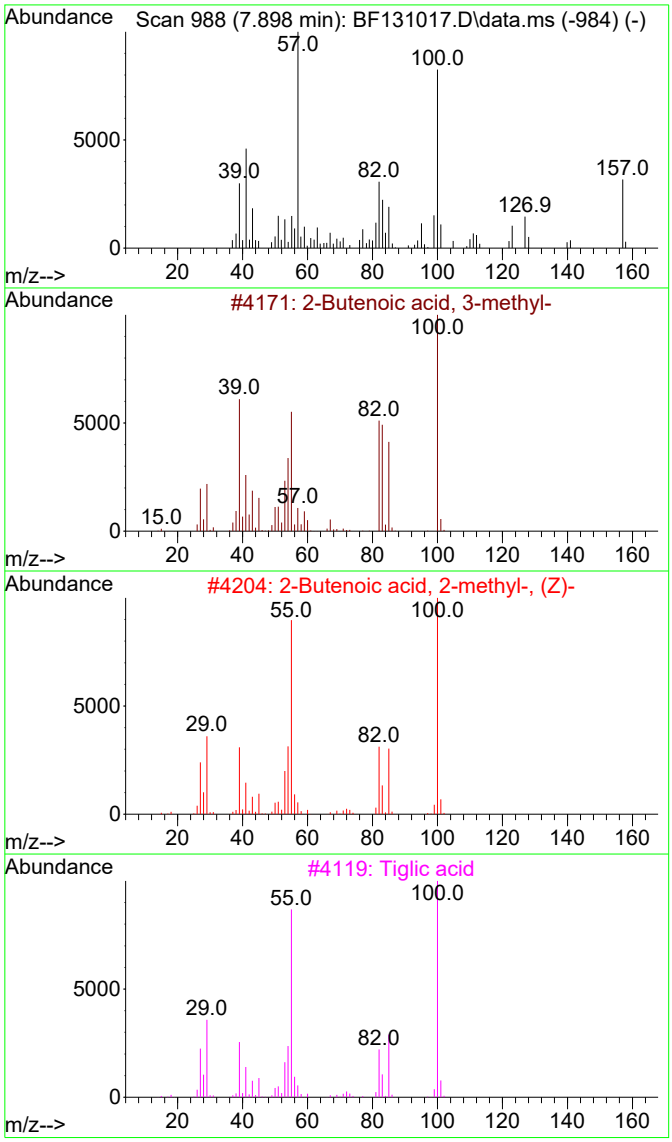
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

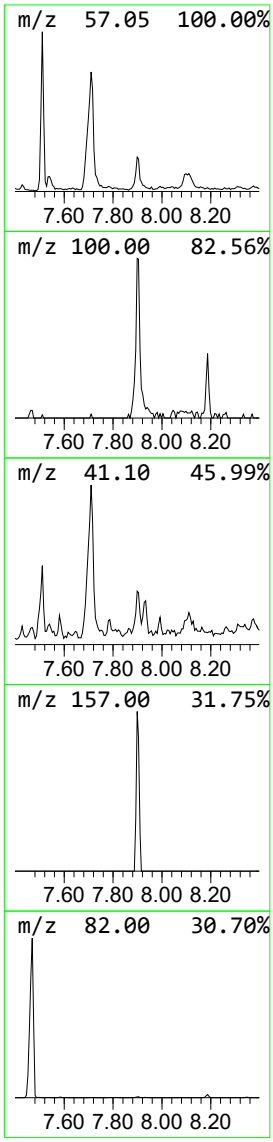
****

Peak Number 5 2-Butenoic acid, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.898	2.54 ng	62309	Naphthalene-d8	8.187

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenoic acid, 3-methyl-	100	C5H8O2	000541-47-9	50
2	2-Butenoic acid, 2-methyl-, (Z)-	100	C5H8O2	000565-63-9	47
3	Tiglic acid	100	C5H8O2	000080-59-1	47
4	5-Heptenoic acid, 2,6-dimethyl-2...	182	C11H18O2	100052-75-3	38
5	Methylphosphonic difluoride	100	CH3F2OP	000676-99-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131017.D
Acq On : 05 Nov 2022 13:42
Operator : CG\JU
Sample : N5340-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-8-102722

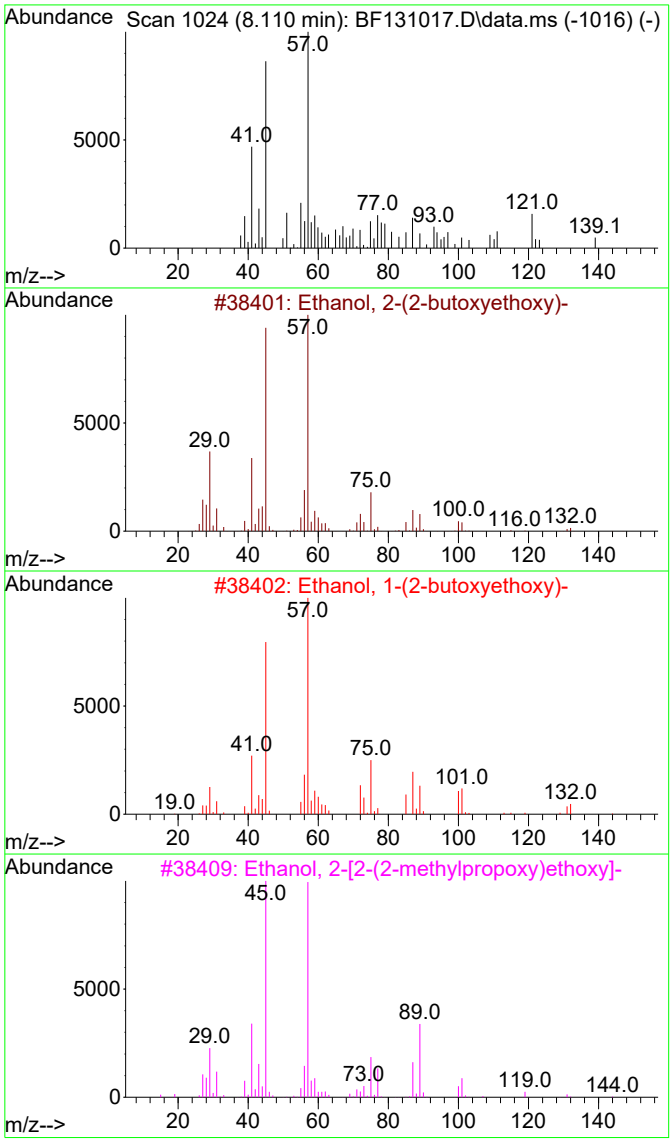
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

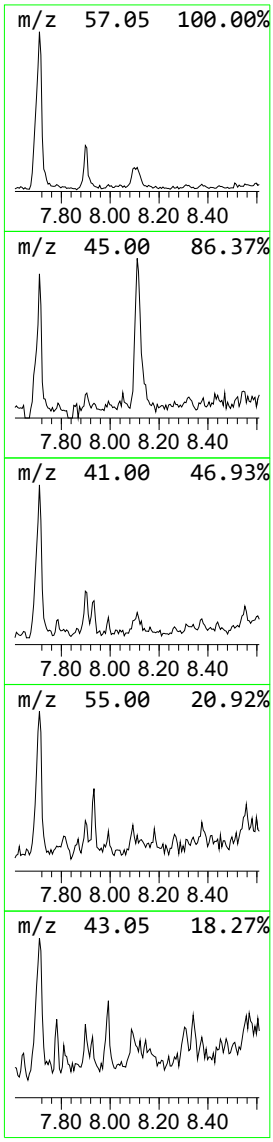
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	2.46 ng	60480	Naphthalene-d8	8.187

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	59
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	45
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	45
4	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	42
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	40





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Data File : BF131017.D
Acq On : 05 Nov 2022 13:42
Operator : CG\JU
Sample : N5340-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-8-102722

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

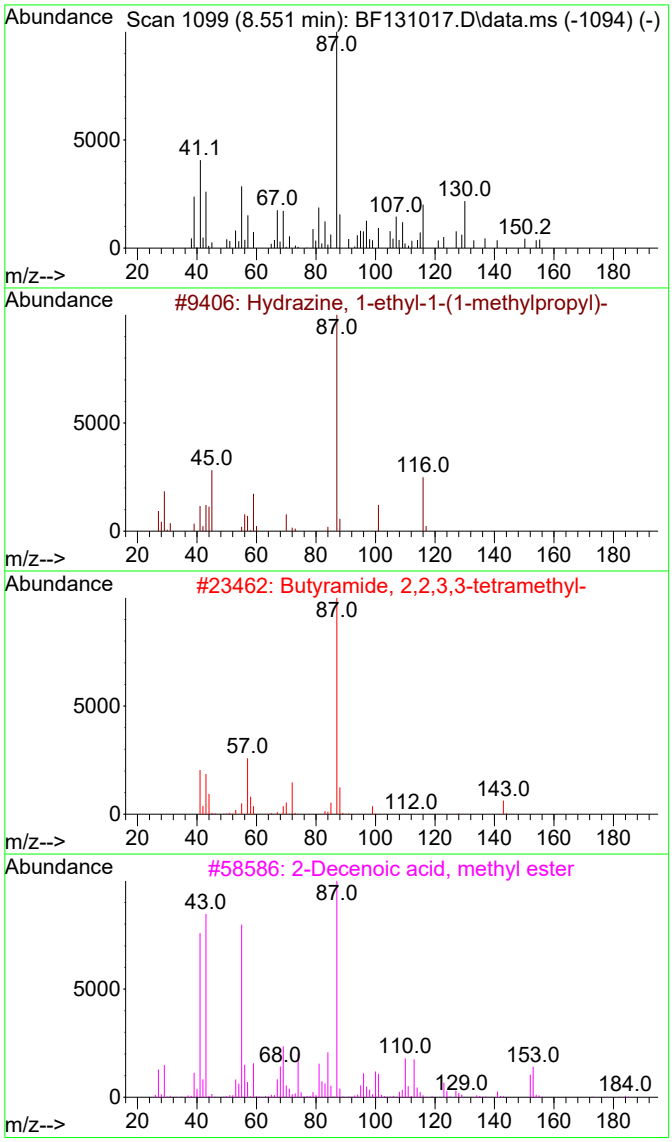
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

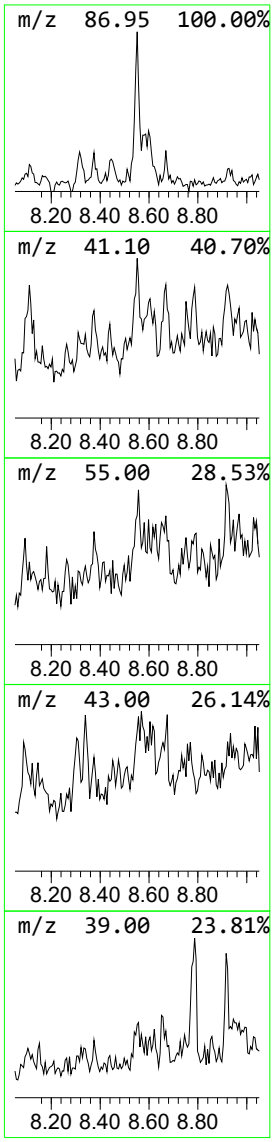
****

Peak Number 7 unknown8.551 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.551	2.01 ng	49280	Naphthalene-d8	8.187

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazine, 1-ethyl-1-(1-methylpr...	116	C6H16N2	020325-97-7	47
2	Butyramide, 2,2,3,3-tetramethyl-	143	C8H17NO	098486-62-5	38
3	2-Decenoic acid, methyl ester	184	C11H20O2	002482-39-5	38
4	Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	37
5	Thiophane, propyl-	130	C7H14S	001551-34-4	37





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Data File : BF131017.D
Acq On : 05 Nov 2022 13:42
Operator : CG\JU
Sample : N5340-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-8-102722

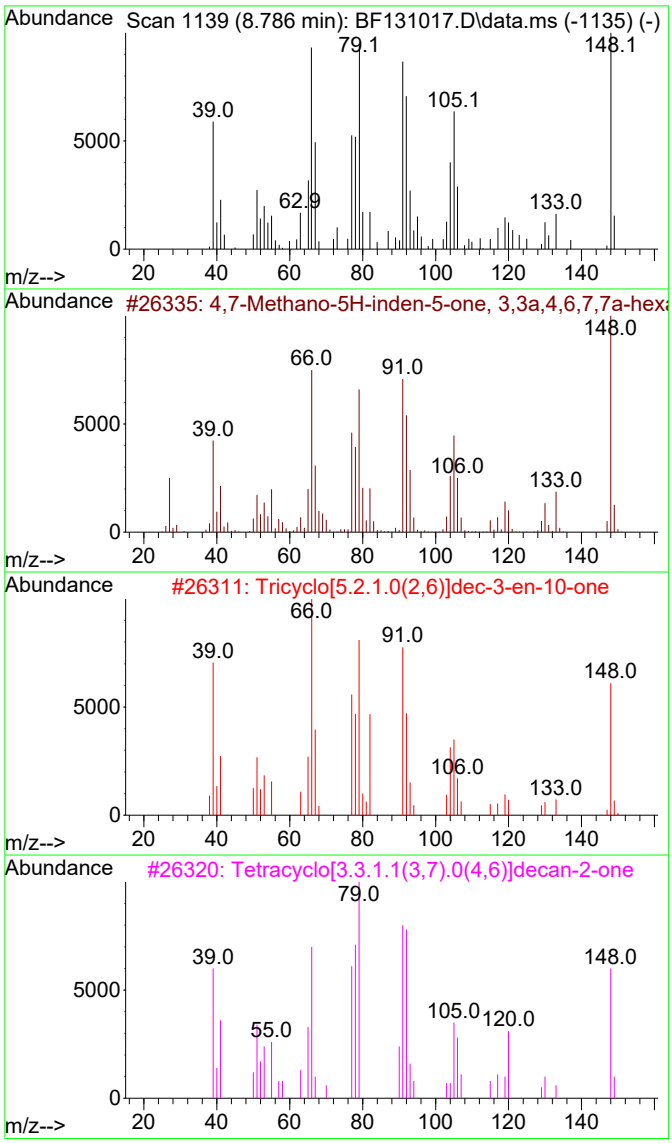
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

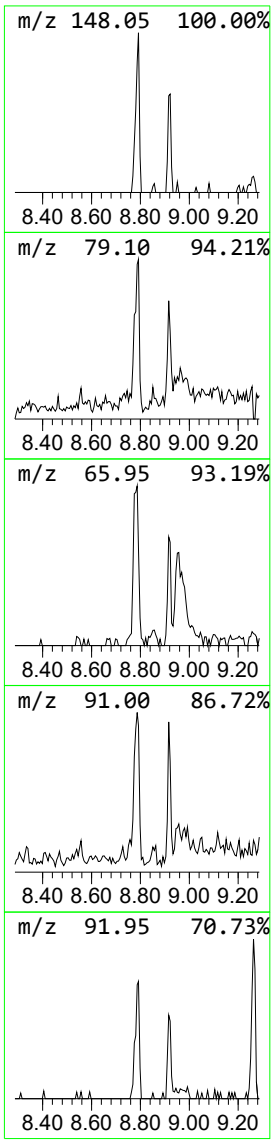
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 4,7-Methano-5H-inden-5-one,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.786	2.95 ng	72509	Naphthalene-d8	8.187

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,7-Methano-5H-inden-5-one, 3,3a...	148	C10H12O	014888-58-5	96
2	Tricyclo[5.2.1.0(2,6)]dec-3-en-1...	148	C10H12O	1000289-10-5	94
3	Tetracyclo[3.3.1.1(3,7).0(4,6)]d...	148	C10H12O	052750-53-5	64
4	6(5H)-Pteridinone	148	C6H4N4O	002432-26-0	60
5	Bicyclo[2.2.1]hept-2-ene, 5-meth...	106	C8H10	000694-91-7	55





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Acq On : 05 Nov 2022 13:42
Operator : CG\JU
Sample : N5340-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-8-102722

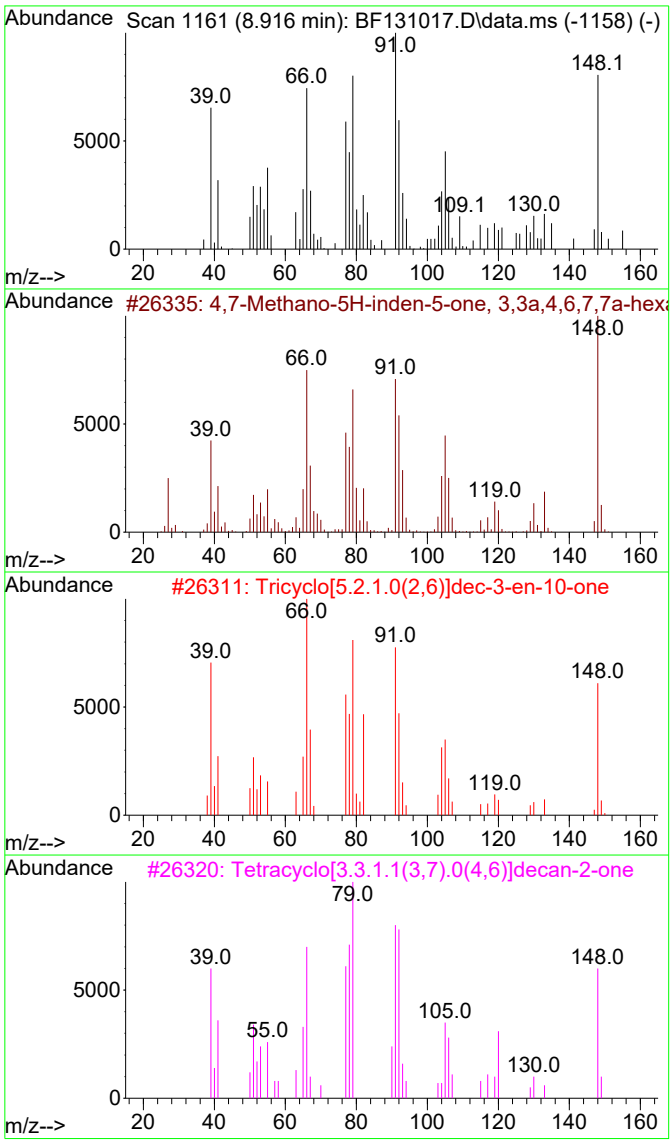
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

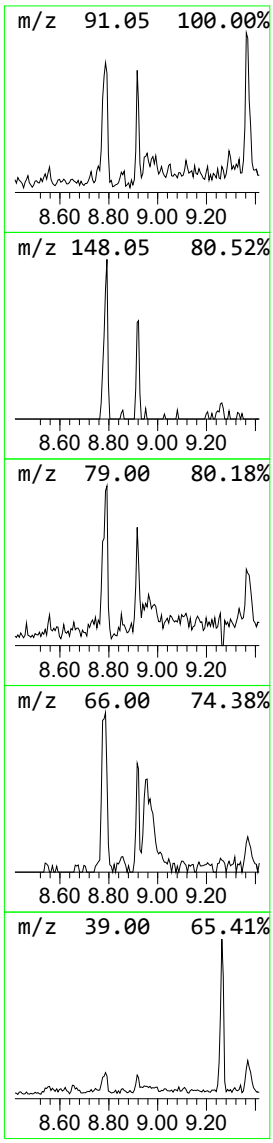
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Tricyclo[5.2.1.0(2,6)]dec-3... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.916	2.11 ng	51755	Naphthalene-d8	8.187

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,7-Methano-5H-inden-5-one, 3,3a...	148	C10H12O	014888-58-5	98
2	Tricyclo[5.2.1.0(2,6)]dec-3-en-1...	148	C10H12O	1000289-10-5	91
3	Tetracyclo[3.3.1.1(3,7).0(4,6)]d...	148	C10H12O	052750-53-5	72
4	1H-Indene, 3a,4,7,7a-tetrahydro-...	120	C9H12	066563-20-0	50
5	Bicyclo[2.2.1]hept-2-ene, 5-meth...	106	C8H10	000694-91-7	46





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Operator : CG\JU
Sample : N5340-04
Misc :
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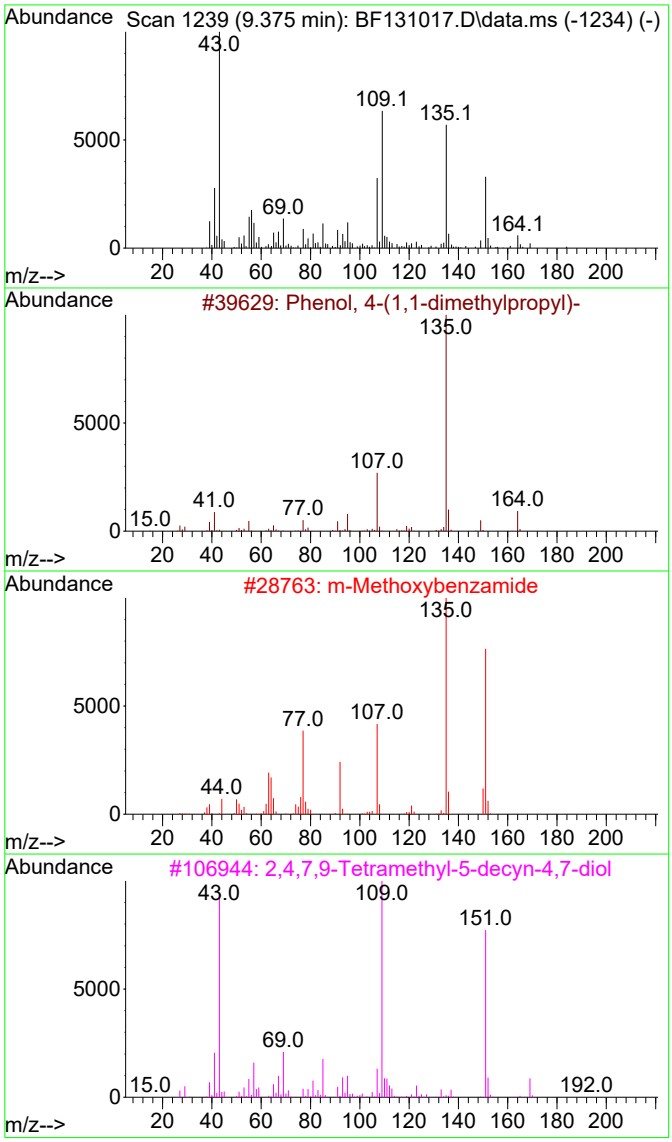
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

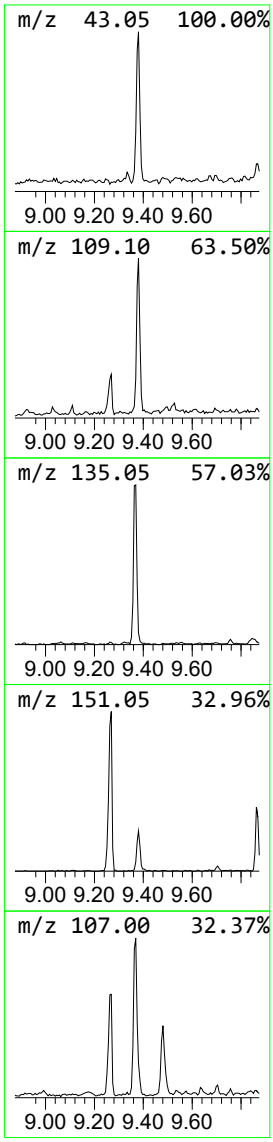
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Phenol, 4-(1,1-dimethylprop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.375	10.41 ng	287126	Acenaphthene-d10	9.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	64
2	m-Methoxybenzamide	151	C8H9NO2	005813-86-5	46
3	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	46
4	Pyridine, 3-butyl-, 1-oxide	151	C9H13NO	031396-33-5	38
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	35





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-8-102722

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
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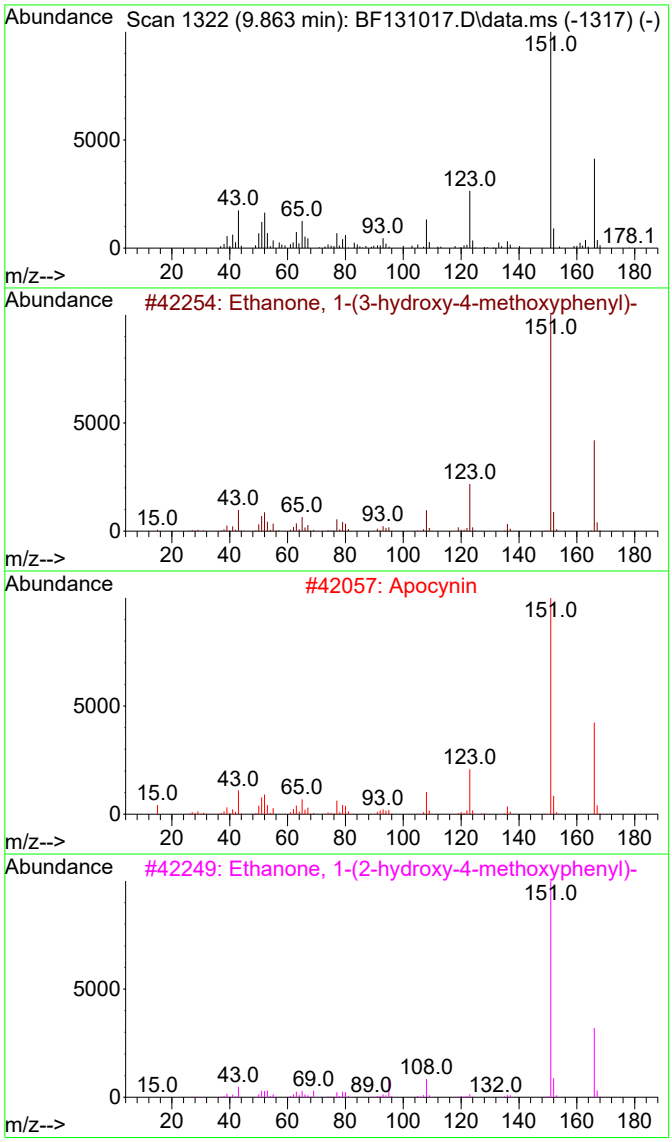
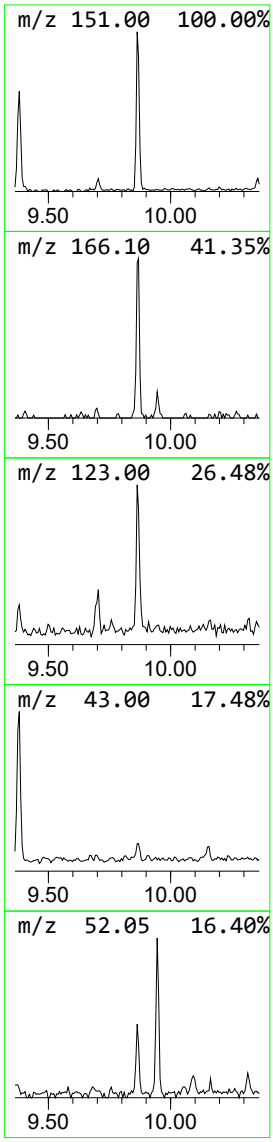
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Ethanone, 1-(3-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.863	4.35 ng	119844	Acenaphthene-d10	9.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(3-hydroxy-4-methoxy...	166	C9H10O3	006100-74-9	94
2	Apocynin	166	C9H10O3	000498-02-2	94
3	Ethanone, 1-(2-hydroxy-4-methoxy...	166	C9H10O3	000552-41-0	72
4	Ethanone, 1-(2-hydroxy-6-methoxy...	166	C9H10O3	000703-23-1	72
5	t-Butylhydroquinone	166	C10H14O2	001948-33-0	72





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

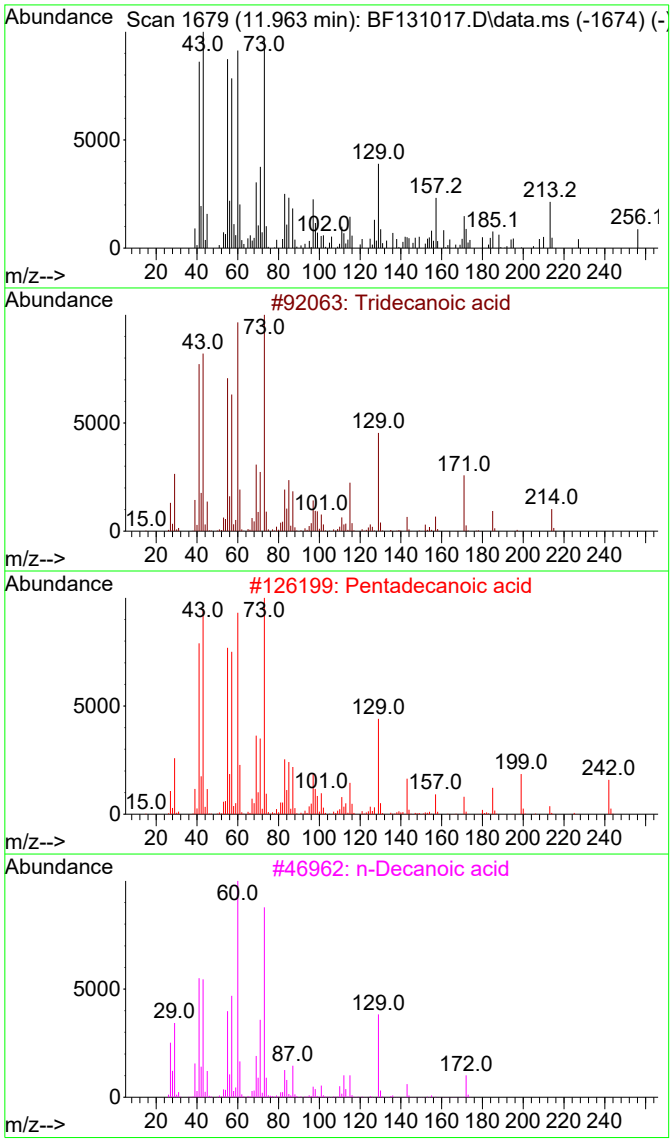
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

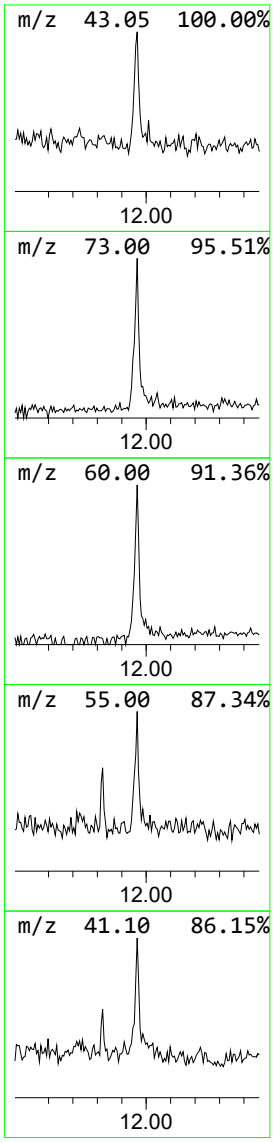
****

Peak Number 12 Tridecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.963	2.67 ng	65111	Phenanthrene-d10	11.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	n-Decanoic acid	172	C10H20O2	000334-48-5	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-8-102722

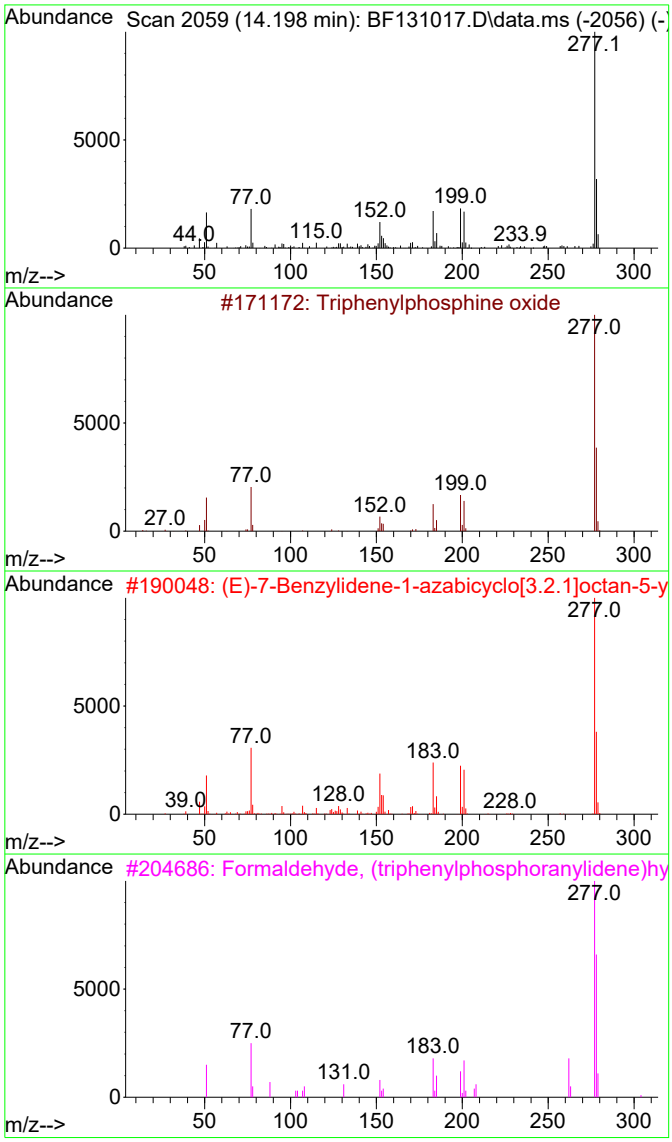
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

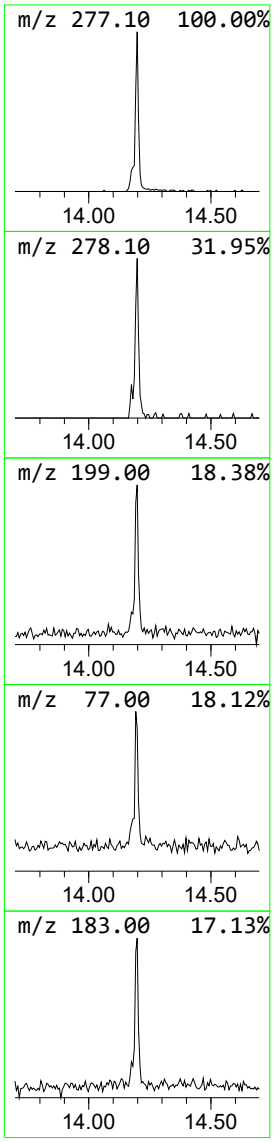
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.198	3.54 ng	61103	Chrysene-d12	14.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	58
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	42
5	1H-Indole-3-acetic acid, 5-[(tri...	277	C14H19NO3Si	072101-35-0	38





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
Butane, 2-metho...	2.193	85.9	ng	1640020	1	6.904	381822	20.0
2-Pentanone, 4-...	5.122	8.9	ng	170516	1	6.904	381822	20.0
Phorone	7.581	2.7	ng	66457	2	8.187	491559	20.0
Hexanoic acid, ...	7.710	8.2	ng	202167	2	8.187	491559	20.0
2-Butenoic acid...	7.898	2.5	ng	62309	2	8.187	491559	20.0
Ethanol, 2-(2-b...	8.110	2.5	ng	60480	2	8.187	491559	20.0
unknown8.551	8.551	2.0	ng	49280	2	8.187	491559	20.0
4,7-Methano-5H-...	8.786	3.0	ng	72509	2	8.187	491559	20.0
Tricyclo[5.2.1....	8.916	2.1	ng	51755	2	8.187	491559	20.0
Phenol, 4-(1,1-...	9.375	10.4	ng	287126	3	9.945	551397	20.0
Ethanone, 1-(3-...	9.863	4.3	ng	119844	3	9.945	551397	20.0
Tridecanoic acid	11.963	2.7	ng	65111	4	11.439	487682	20.0
Triphenylphosph...	14.198	3.5	ng	61103	5	14.086	344976	20.0