LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
Data File : BF126061.D
Acq On : 8 Nov 2021 12:55
Operator : JU/CG
Sample : M4500-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-8-110321

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-BF110321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126061.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.151	3	11	17	rBV	1708888	2108909	47.44%	6.165%
2	3.345	209	214	225	rBV	104985	211916	4.77%	0.620%
3	5.069	496	507	513	rBV	105560	131776	2.96%	0.385%
4	5.469	570	575	578	rBV	3767601	3554674	79.95%	10.392%
5	6.481	741	747	750	rBV	3883245	3733246	83.97%	10.914%
6	6.851	807	810	814	rBV	1299931	1014841	22.83%	2.967%
7	7.416	900	906	909	rBV	2439587	2458186	55.29%	7.186%
8	8.039	1008	1012	1023	rBV	247654	301987	6.79%	0.883%
9	8.133	1023	1028	1031	rBV	1600852	1313052	29.53%	3.839%
10	9.157	1200	1202	1206	rBV2	62796	61597	1.39%	0.180%
11	9.210	1206	1211	1214	rBV	5695214	4445892	100.00%	12.997%
12	9.292	1222	1225	1229	rBV3	65540	71313	1.60%	0.208%
13	9.410	1241	1245	1250	rVB2	38596	62042	1.40%	0.181%
14	9.469	1250	1255	1259	rBV2	73634	97083	2.18%	0.284%
15	9.545	1265	1268	1270	rBV2	85251	78415	1.76%	0.229%
16	9.616	1275	1280	1282	rVV3	68492	80356	1.81%	0.235%
17	9.663	1285	1288	1293	rVB2	62181	70632	1.59%	0.206%
18	9.745	1300	1302	1307	rVB3	65523	67751	1.52%	0.198%
19	9.886	1320	1326	1329	rBV	1740303	1428556	32.13%	4.176%
20	9.916	1329	1331	1335	rVB2	90025	95232	2.14%	0.278%
21	9.992	1341	1344	1348	rVB3	43925	63641	1.43%	0.186%
22	10.045	1348	1353	1357	rBV4	33879	55723	1.25%	0.163%
23	10.086	1357	1360	1364	rVB2	89565	89571	2.01%	0.262%
24	10.292	1391	1395	1398	rBV	92421	115181	2.59%	0.337%
25	10.433	1415	1419	1425	rBV3	84368	103730	2.33%	0.303%
26	10.498	1425	1430	1432	rBV2	50055	56534	1.27%	0.165%
27	10.592	1443	1446	1450	rVB4	51542	60353	1.36%	0.176%
28	10.674	1455	1460	1463	rBV	2764989	2391145	53.78%	6.990%
29	10.792	1477	1480	1485	rVB4	79362	116999	2.63%	0.342%
30	11.116	1529	1535	1542	rBV	215961	285881	6.43%	0.836%
31	11.269	1559	1561	1566	rVB2	98676	97667	2.20%	0.286%
32	11.369	1575	1578	1581	rBV	1369353	1225919	27.57%	3.584%
33	11.392	1581	1582	1585	rVV	282304	178231	4.01%	0.521%
34	11.445	1585	1591	1594	rVB	144582	176956	3.98%	0.517%
35	11.668	1626	1629	1632	rBV	69589	56339	1.27%	0.165%
36	11.768	1643	1646	1653	rVB2	114041	116327	2.62%	0.340%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
Data File : BF126061.D
Acq On : 8 Nov 2021 12:55
Operator : JU/CG
Sample : M4500-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-8-110321

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-BF110321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.874	1661	1664	1666	rBV	94480	89328	2.01%	0.261%
38	11.898	1666	1668	1671	rVB	160269	129803	2.92%	0.379%
39	11.980	1679	1682	1685	rBV2	143912	168068	3.78%	0.491%
40	12.074	1696	1698	1701	rBV	68584	61486	1.38%	0.180%
41	12.357	1742	1746	1751	rBV6	42453	80952	1.82%	0.237%
42	12.427	1755	1758	1760	rVV	79958	74325	1.67%	0.217%
43	12.474	1760	1766	1769	rVV3	149480	291210	6.55%	0.851%
44	12.586	1782	1785	1787	rBV	291965	233831	5.26%	0.684%
45	12.810	1820	1823	1826	rBV	321049	265572	5.97%	0.776%
46	12.833	1826	1827	1830	rVB	85020	63824	1.44%	0.187%
47	12.957	1844	1848	1851	rBV	4007948	3331486	74.93%	9.739%
48	13.027	1858	1860	1864	rBV3	38471	58171	1.31%	0.170%
49	13.139	1877	1879	1882	rVB	122003	100210	2.25%	0.293%
50	13.192	1885	1888	1893	rBV3	61276	101340	2.28%	0.296%
51	13.498	1937	1940	1944	rBV	234464	219299	4.93%	0.641%
52	13.533	1944	1946	1949	rVV2	65678	70350	1.58%	0.206%
53	13.874	2000	2004	2013	rVB5	170825	330878	7.44%	0.967%
54	14.010	2022	2027	2030	rBV	1076455	1072314	24.12%	3.135%
55	14.486	2106	2108	2110	rVB2	101165	75257	1.69%	0.220%
56	15.474	2272	2276	2280	rBV	701436	811324	18.25%	2.372%

Sum of corrected areas: 34206681

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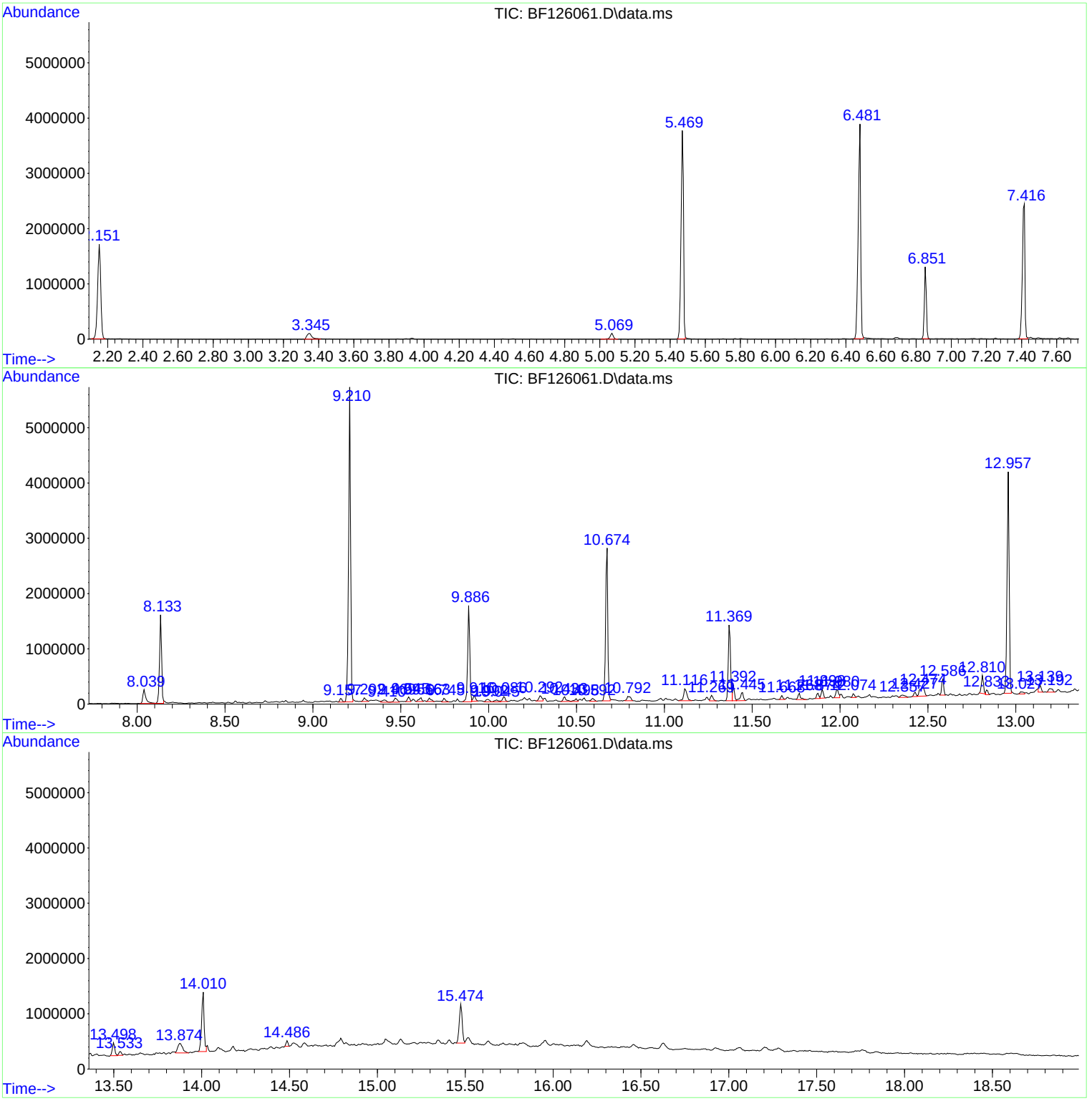
Acq On : 8 Nov 2021 12:55
Operator : JU/CG
Sample : M4500-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-8-110321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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\BF110821\
Data File : BF126061.D
Acq On : 8 Nov 2021 12:55
Operator : JU/CG
Sample : M4500-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-8-110321

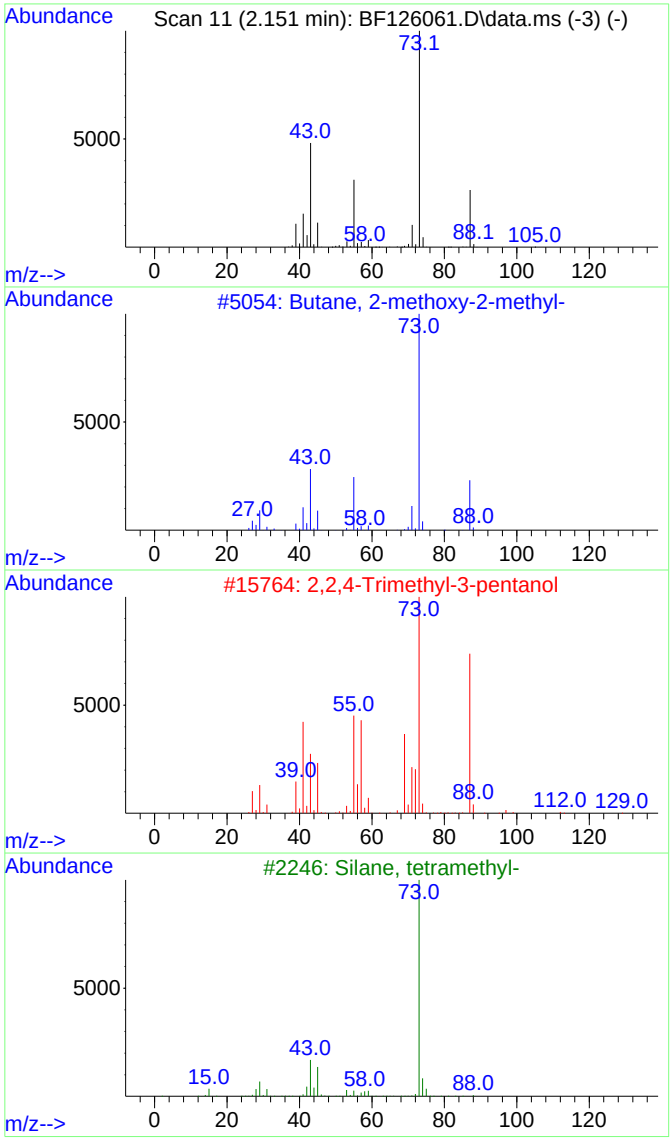
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

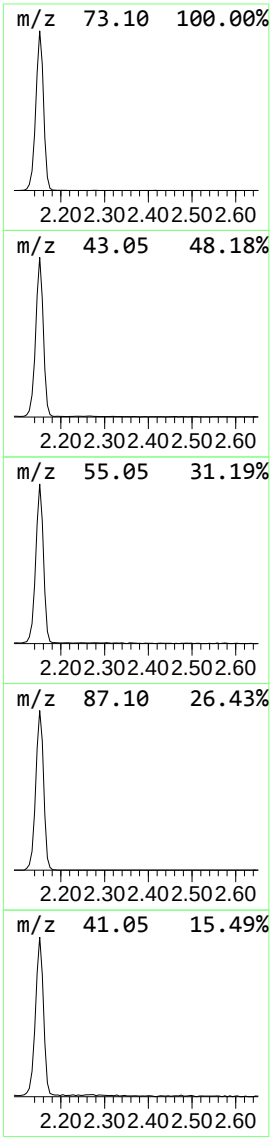
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.151	41.56 ng	2108910	1,4-Dichlorobenzene-d4	6.851

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
Data File : BF126061.D
Acq On : 8 Nov 2021 12:55
Operator : JU/CG
Sample : M4500-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-8-110321

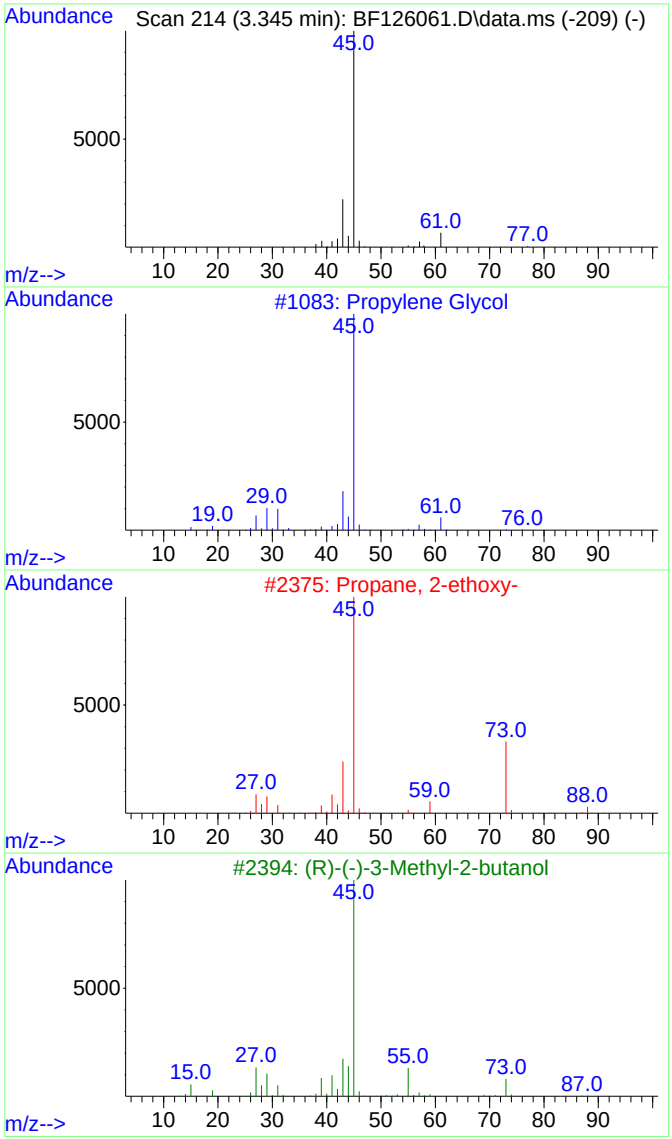
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

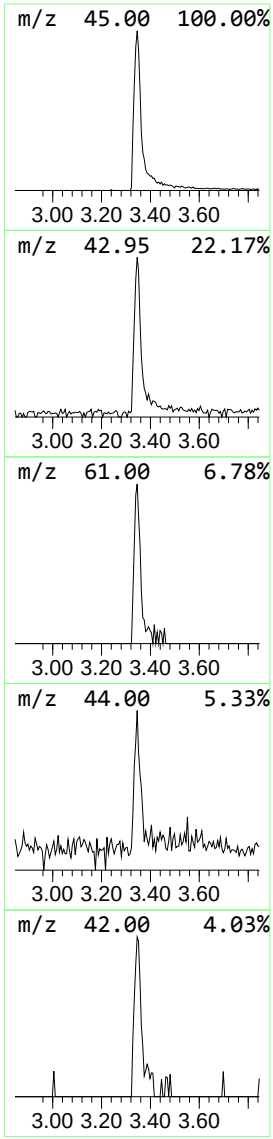
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 unknown3.345 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.345	4.18 ng	211916	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	43
2	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9
3	(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
Data File : BF126061.D
Acq On : 8 Nov 2021 12:55
Operator : JU/CG
Sample : M4500-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-8-110321

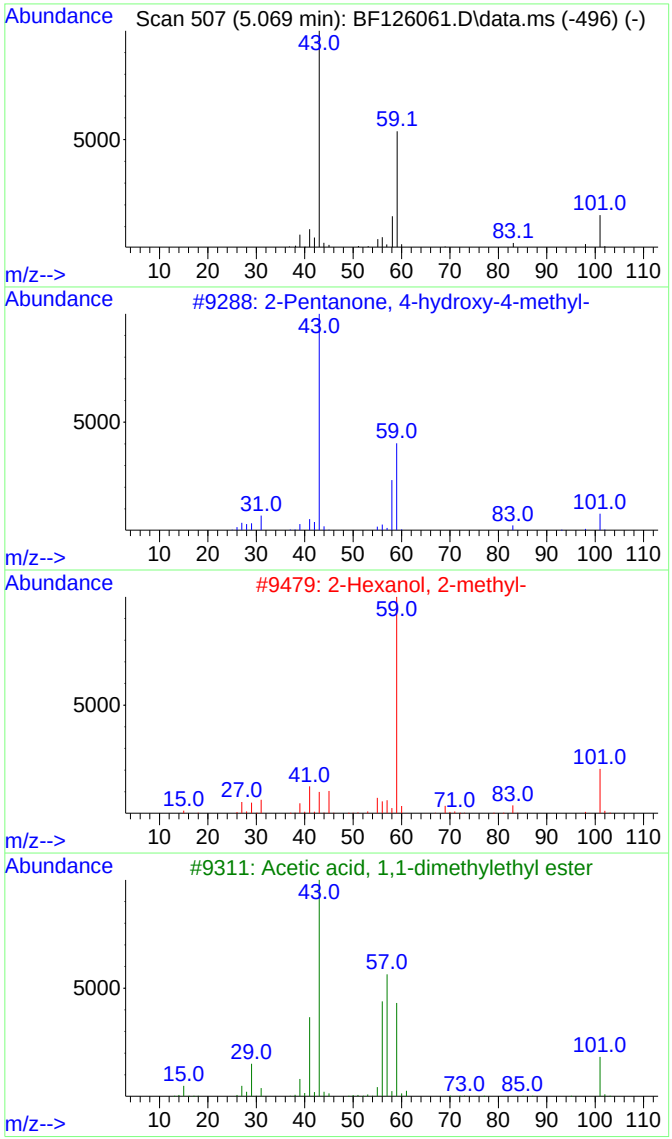
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

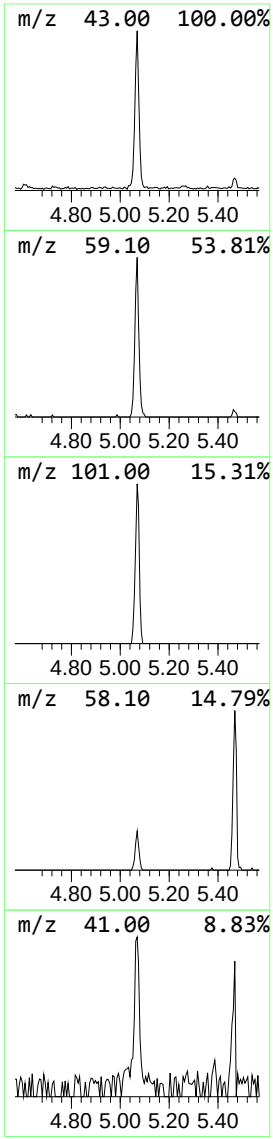
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	2.60 ng	131776	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	3-Octanol	130	C8H18O	000589-98-0	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
Data File : BF126061.D
Acq On : 8 Nov 2021 12:55
Operator : JU/CG
Sample : M4500-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-8-110321

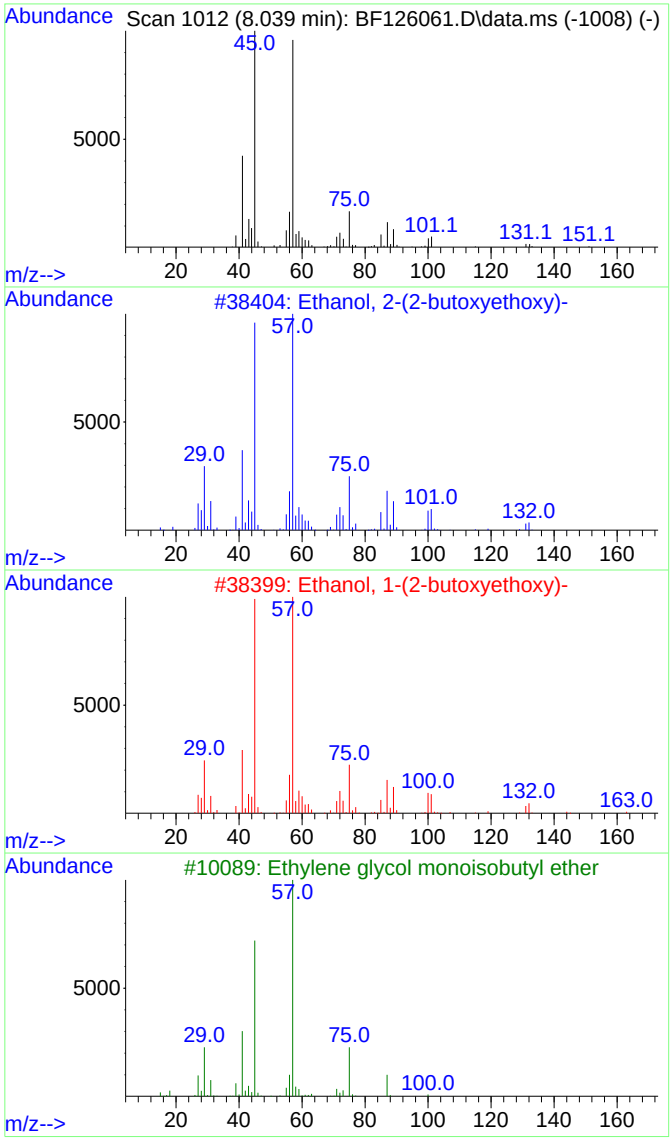
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

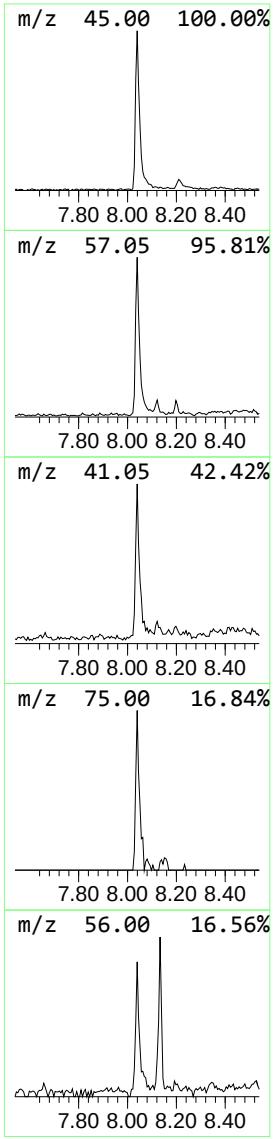
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.039	4.60 ng	301987	Naphthalene-d8	8.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	53
5	Pentaethylene glycol	238	C10H22O6	004792-15-8	50





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Data File : BF126061.D
Acq On : 8 Nov 2021 12:55
Operator : JU/CG
Sample : M4500-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-8-110321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

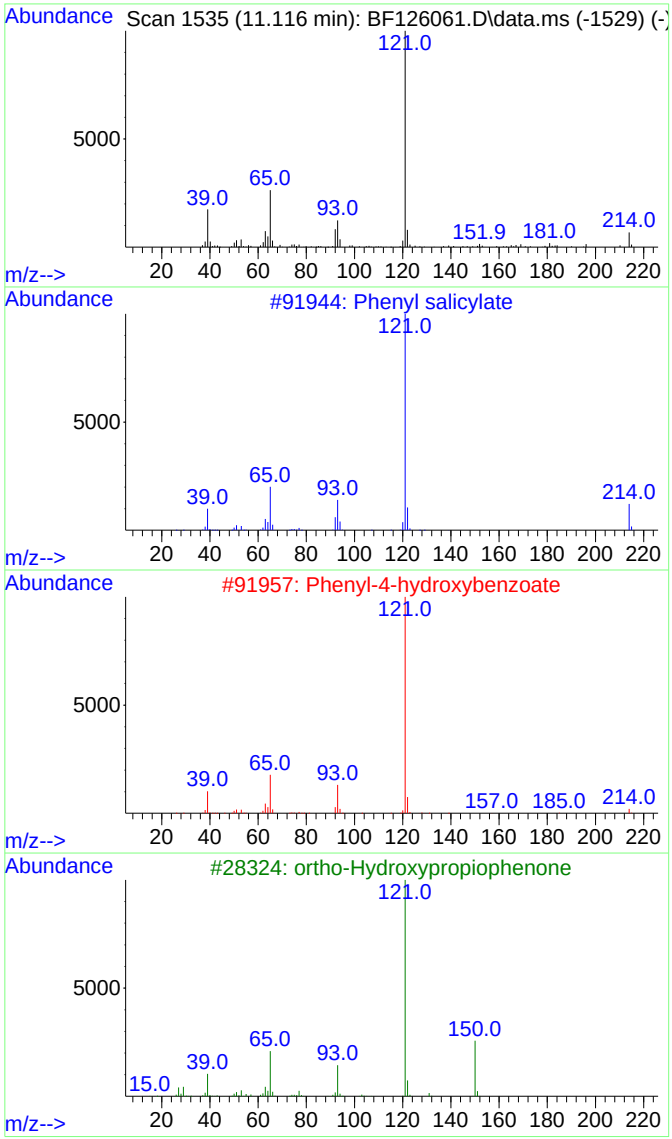
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

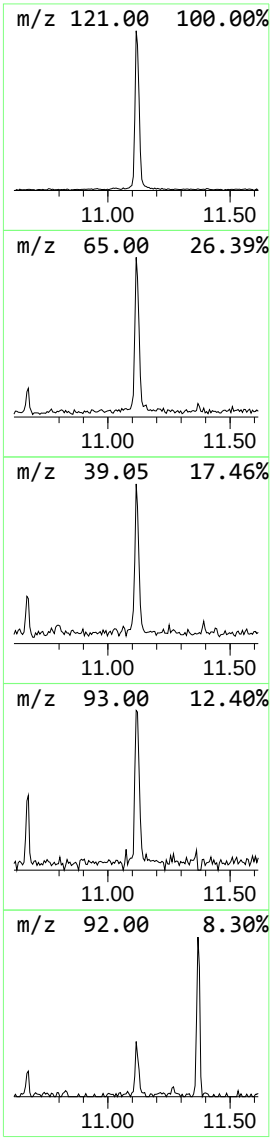
****

Peak Number 5 Phenyl salicylate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.116	4.66 ng	285881	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenyl salicylate	214	C13H10O3	000118-55-8	97
2	Phenyl-4-hydroxybenzoate	214	C13H10O3	017696-62-7	91
3	ortho-Hydroxypropiophenone	150	C9H10O2	000610-99-1	72
4	Salicyl hydrazide	152	C7H8N2O2	000936-02-7	64
5	N-Cyclopropyl-2-hydroxybenzamide	177	C10H11NO2	440111-82-0	64





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Data File : BF126061.D
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Sample : M4500-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-8-110321

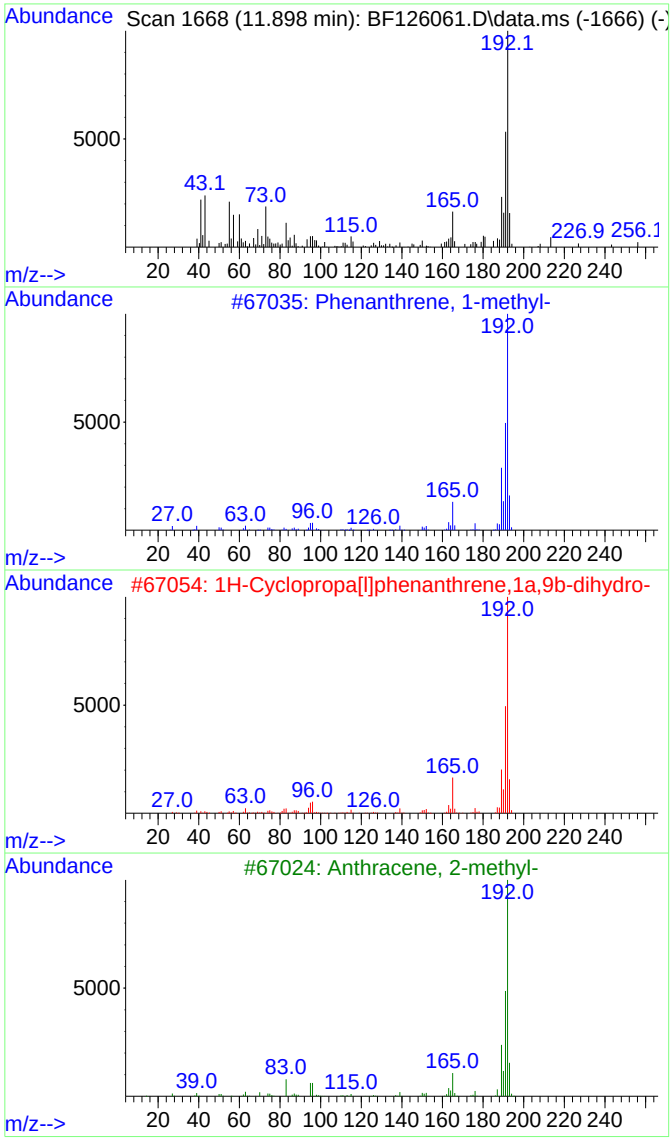
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

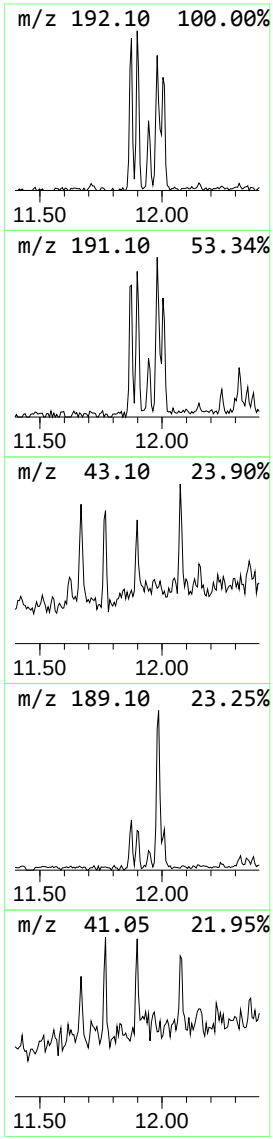
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Phenanthrene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	2.12 ng	129803	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
2	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	94
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	89
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	76





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Data File : BF126061.D
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-8-110321

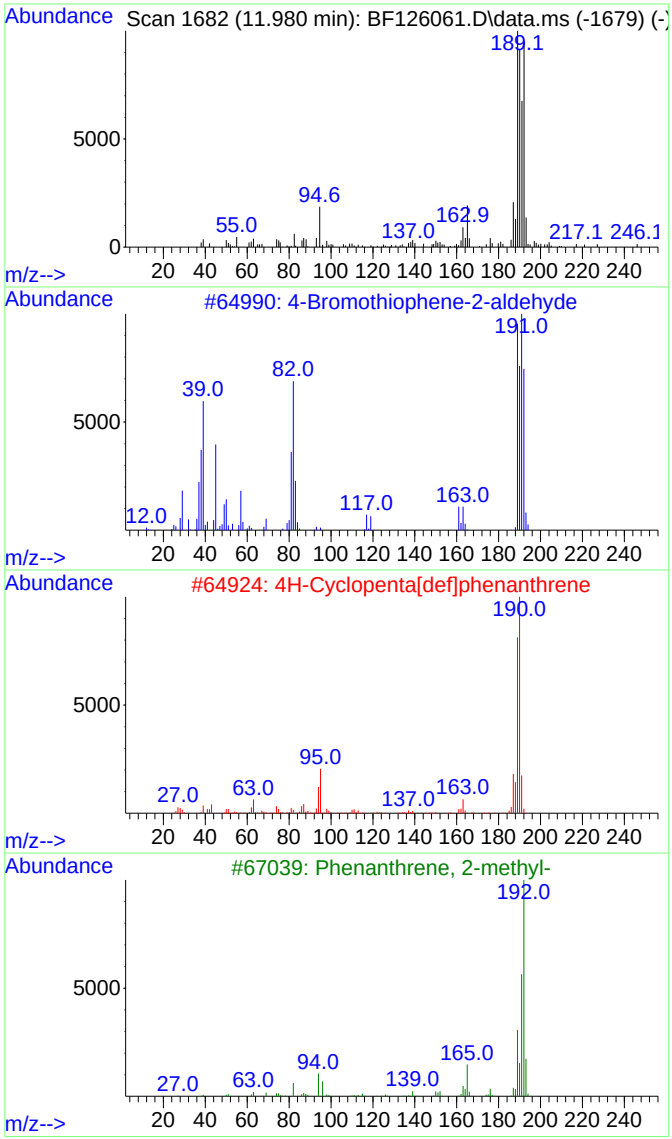
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

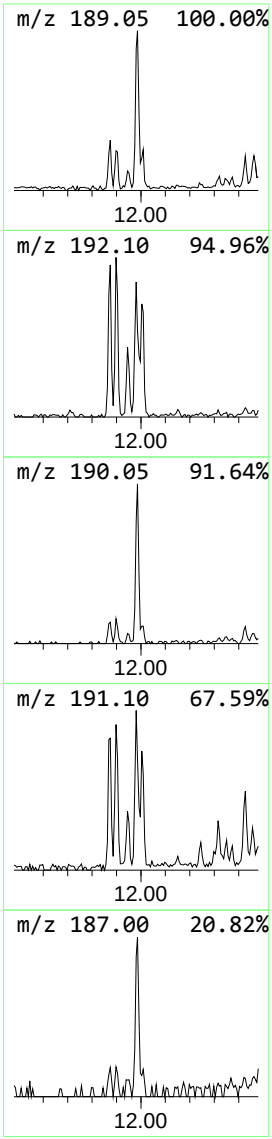
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 4-Bromothiophene-2-aldehyde Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.980	2.74 ng	168068	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	58
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	49
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	46
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	46
5	1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
Data File : BF126061.D
Acq On : 8 Nov 2021 12:55
Operator : JU/CG
Sample : M4500-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-8-110321

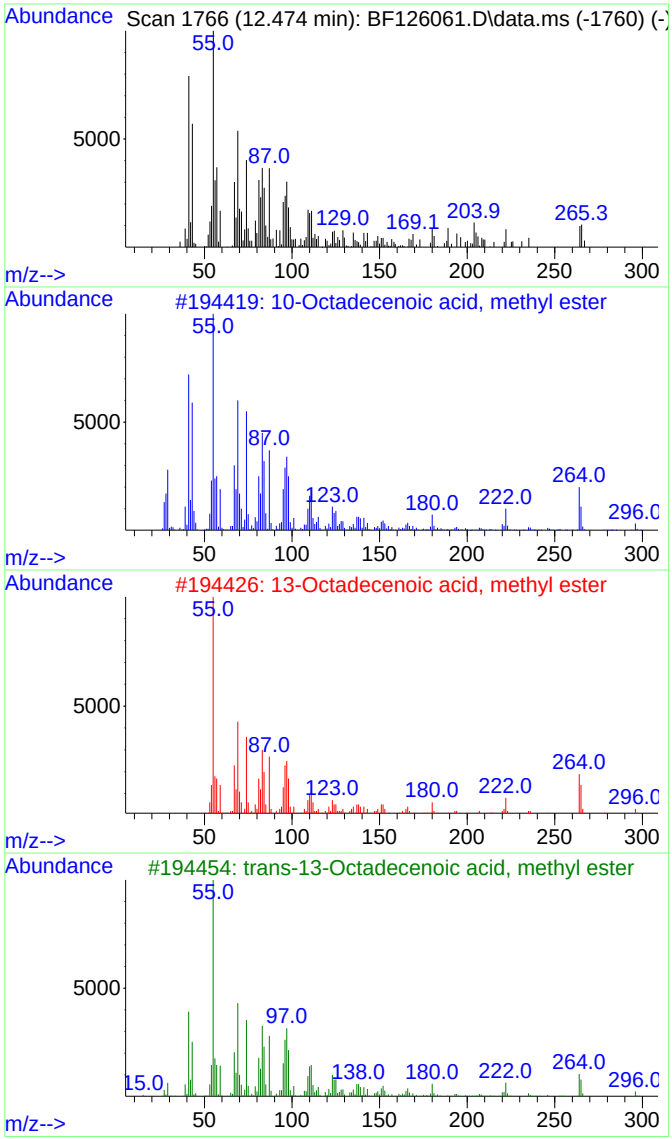
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

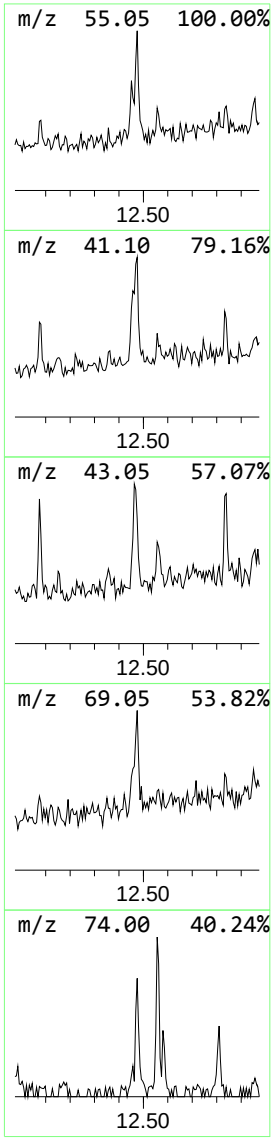
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 10-Octadecenoic acid, methy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.474	4.75 ng	291210	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	87
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	87
3	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	86
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	86
5	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	81





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Data File : BF126061.D
Acq On : 8 Nov 2021 12:55
Operator : JU/CG
Sample : M4500-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-8-110321

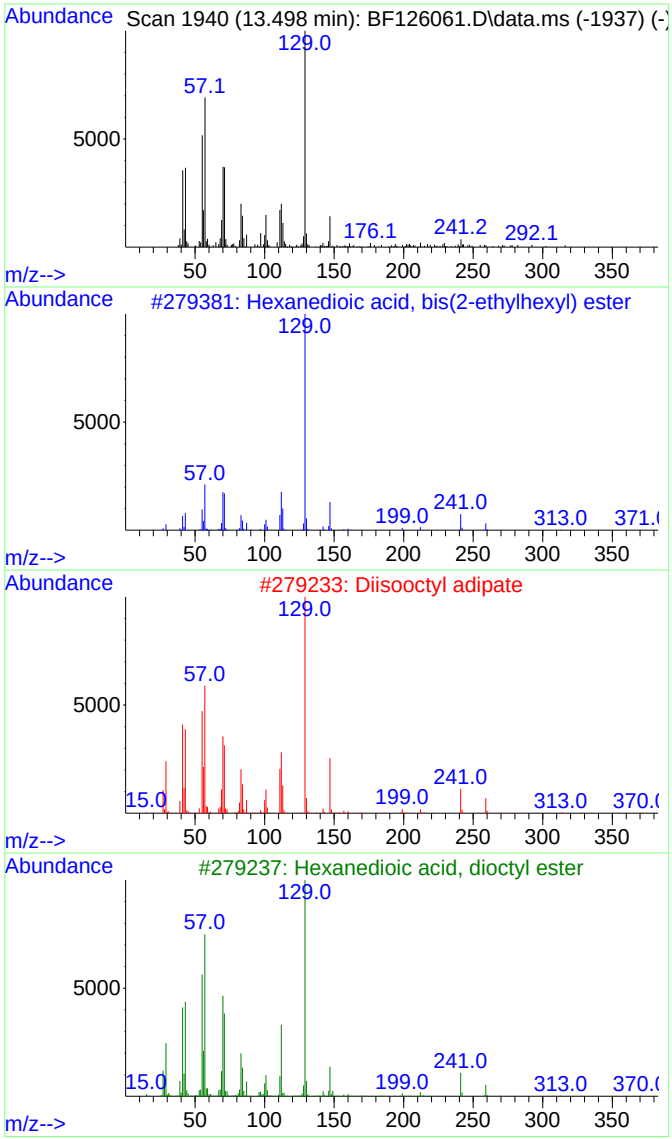
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

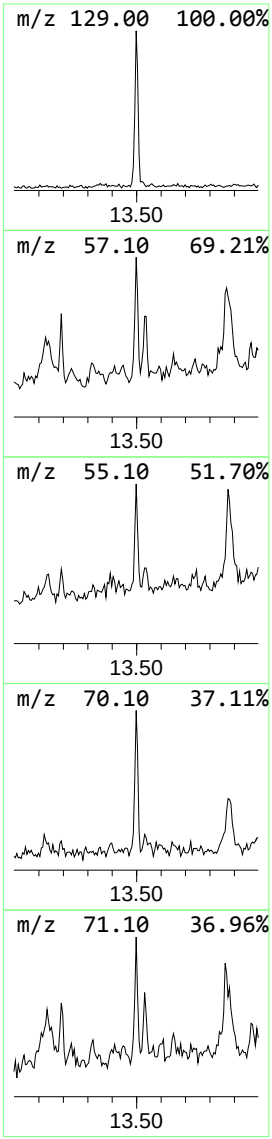
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Hexanedioic acid, bis(2-eth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.498	4.09 ng	219299	Chrysene-d12	14.009

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	86
2	Diisooctyl adipate	370	C22H42O4	001330-86-5	72
3	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	72
4	Adipic acid, 2-ethylhexyl nonyl ...	384	C23H44O4	1000324-48-7	64
5	Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
Data File : BF126061.D
Acq On : 8 Nov 2021 12:55
Operator : JU/CG
Sample : M4500-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-8-110321

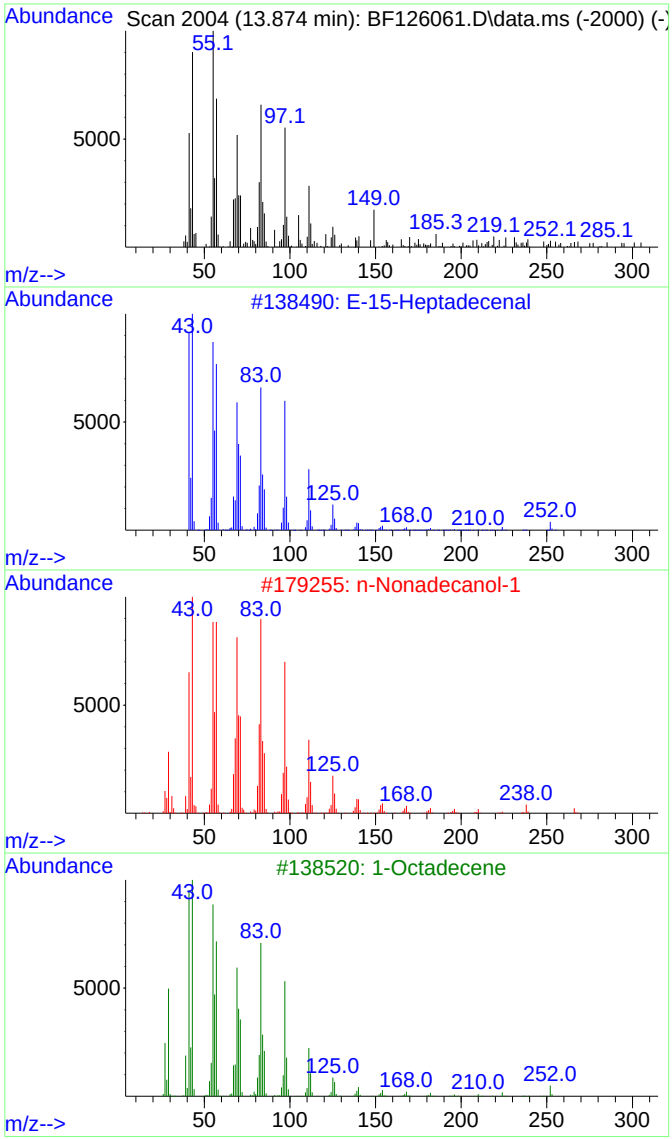
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

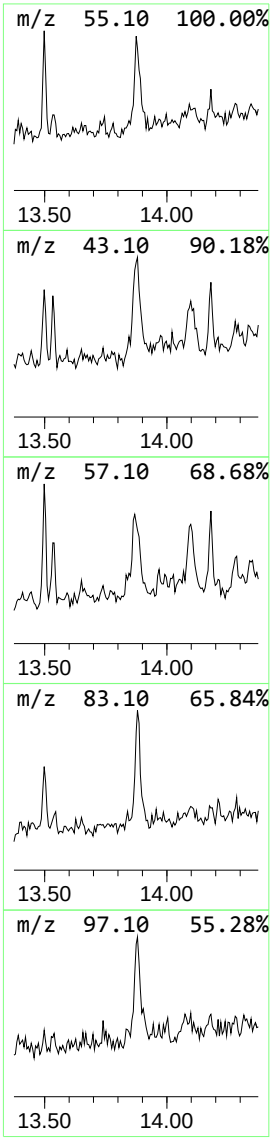
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 E-15-Heptadecenal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	6.17 ng	330878	Chrysene-d12	14.009

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	96
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
3	1-Octadecene	252	C18H36	000112-88-9	93
4	9-Nonadecene	266	C19H38	031035-07-1	91
5	E-7-Octadecene	252	C18H36	1000130-92-0	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
Data File : BF126061.D
Acq On : 8 Nov 2021 12:55
Operator : JU/CG
Sample : M4500-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-8-110321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
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...	2.151	41.6	ng	2108910	1	6.851	1014840	20.0
unknown3.345	3.345	4.2	ng	211916	1	6.851	1014840	20.0
2-Pentanone, 4-...	5.069	2.6	ng	131776	1	6.851	1014840	20.0
Ethanol, 2-(2-b...	8.039	4.6	ng	301987	2	8.133	1313050	20.0
Phenyl salicylate	11.116	4.7	ng	285881	4	11.368	1225920	20.0
Phenanthrene, 1...	11.898	2.1	ng	129803	4	11.368	1225920	20.0
4-Bromothiophen...	11.980	2.7	ng	168068	4	11.368	1225920	20.0
10-Octadecenoic...	12.474	4.8	ng	291210	4	11.368	1225920	20.0
Hexanedioic aci...	13.498	4.1	ng	219299	5	14.009	1072310	20.0
E-15-Heptadecenal	13.874	6.2	ng	330878	5	14.009	1072310	20.0