LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

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-BF120822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131597.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	4	12	17	rVB	1627640	2053080	81.52%	12.425%
2	3.210	183	191	198	rBV	116309	201607	8.01%	1.220%
3	4.210	356	361	366	rBB	24450	29524	1.17%	0.179%
4	4.398	388	393	397	rBV	30003	35238	1.40%	0.213%
5	5.098	508	512	517	rVB	109733	116821	4.64%	0.707%
6	5.504	577	581	584	rBV	1109277	954035	37.88%	5.774%
7	6.516	749	753	758	rVV	720280	626738	24.89%	3.793%
8	6.569	759	762	766	rVB	81241	68869	2.73%	0.417%
9	6.892	813	817	820	rBV	428132	370354	14.71%	2.241%
10	7.069	836	847	850	rBV	140379	162982	6.47%	0.986%
11	7.134	850	858	860	rVV3	146775	365189	14.50%	2.210%
12	7.157	860	862	869	rVB	156262	149182	5.92%	0.903%
13	7.428	900	908	909	rBV	132775	162945	6.47%	0.986%
14	7.463	909	914	916	rVV	1435797	1608908	63.88%	9.737%
15	7.487	916	918	921	rVB	142831	111576	4.43%	0.675%
16	7.657	945	947	949	rBV	35552	28536	1.13%	0.173%
17	7.687	949	952	955	rVB	92892	69470	2.76%	0.420%
18	7.728	955	959	960	rBV	58755	53641	2.13%	0.325%
19	7.745	960	962	965	rVB	69229	52469	2.08%	0.318%
20	7.910	986	990	994	rBV	107917	109139	4.33%	0.660%
21	8.181	1028	1036	1039	rBV	550680	486382	19.31%	2.944%
22	8.234	1042	1045	1052	rVB5	21212	38361	1.52%	0.232%
23	8.469	1080	1085	1088	rVB3	22625	27575	1.09%	0.167%
24	8.769	1132	1136	1140	rVB2	46487	42575	1.69%	0.258%
25	8.881	1152	1155	1159	rBV2	35544	34809	1.38%	0.211%
26	8.945	1164	1166	1171	rVB3	28959	26065	1.03%	0.158%
27	8.992	1171	1174	1176	rBV	118712	113595	4.51%	0.687%
28	9.039	1176	1182	1184	rVV	211612	344727	13.69%	2.086%
29	9.069	1184	1187	1192	rVB	95098	90676	3.60%	0.549%
30	9.186	1202	1207	1211	rBV	43868	42217	1.68%	0.255%
31	9.263	1214	1220	1223	rBV	2707903	2518474	100.00%	15.241%
32	9.316	1226	1229	1232	rBV	52116	43528	1.73%	0.263%
33	9.457	1249	1253	1258	rVB	219549	208150	8.26%	1.260%
34	9.516	1258	1263	1267	rBV2	129559	149579	5.94%	0.905%
35	9.598	1274	1277	1284	rVB	57426	61473	2.44%	0.372%
36	9.757	1299	1304	1307	rVB2	79914	75332	2.99%	0.456%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

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-BF120822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	9.792	1307	1310	1312	rBV	34423	27776	1.10%	0.168%
38	9.833	1315	1317	1322	rVB2	27392	29778	1.18%	0.180%
39	9.898	1325	1328	1331	rVB2	37398	34254	1.36%	0.207%
40	9.945	1332	1336	1339	rBV	684027	535940	21.28%	3.243%
41	10.280	1388	1393	1396	rBV2	56258	50009	1.99%	0.303%
42	10.416	1412	1416	1419	rVB	68912	55081	2.19%	0.333%
43	10.745	1467	1472	1475	rBV	1592684	1505239	59.77%	9.109%
44	11.439	1587	1590	1594	rVB	569414	521722	20.72%	3.157%
45	11.963	1675	1679	1684	rBV2	26795	31179	1.24%	0.189%
46	13.039	1857	1862	1865	rBV	1506601	1303604	51.76%	7.889%
47	13.998	2020	2025	2038	rBV8	20317	63914	2.54%	0.387%
48	14.098	2038	2042	2046	rVB	350115	317225	12.60%	1.920%
49	14.192	2054	2058	2062	rBV	59306	60800	2.41%	0.368%
50	14.963	2185	2189	2193	rVB	24467	26188	1.04%	0.158%
51	15.610	2293	2299	2308	rBV	253456	327344	13.00%	1.981%

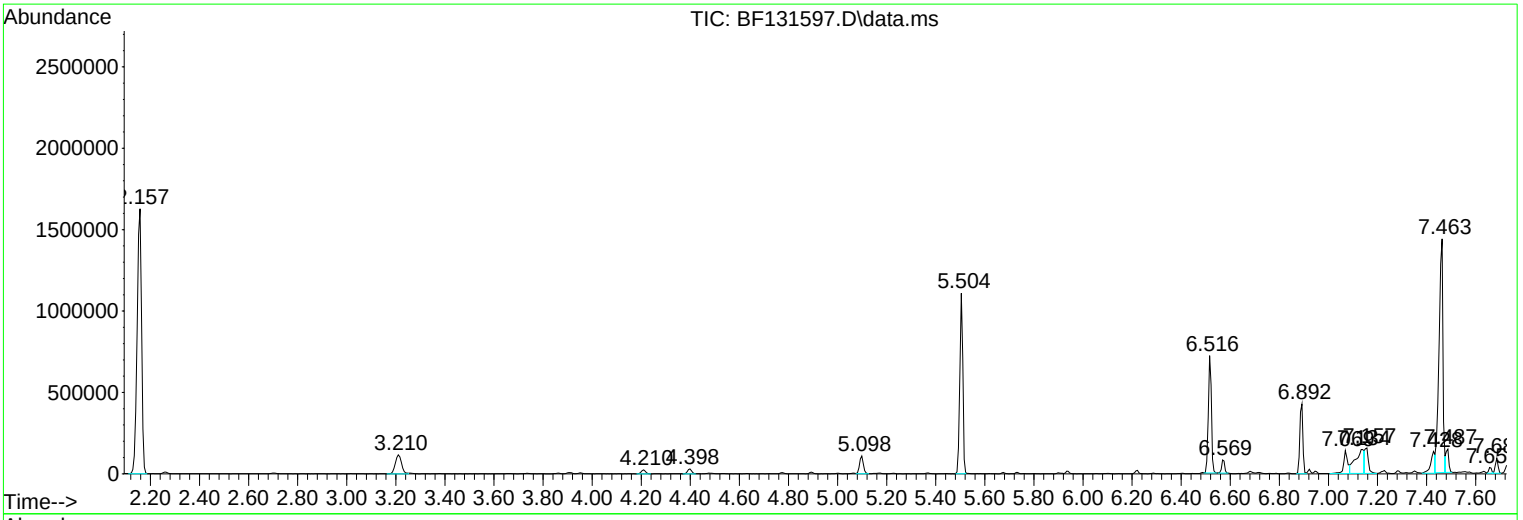
Sum of corrected areas: 16523874

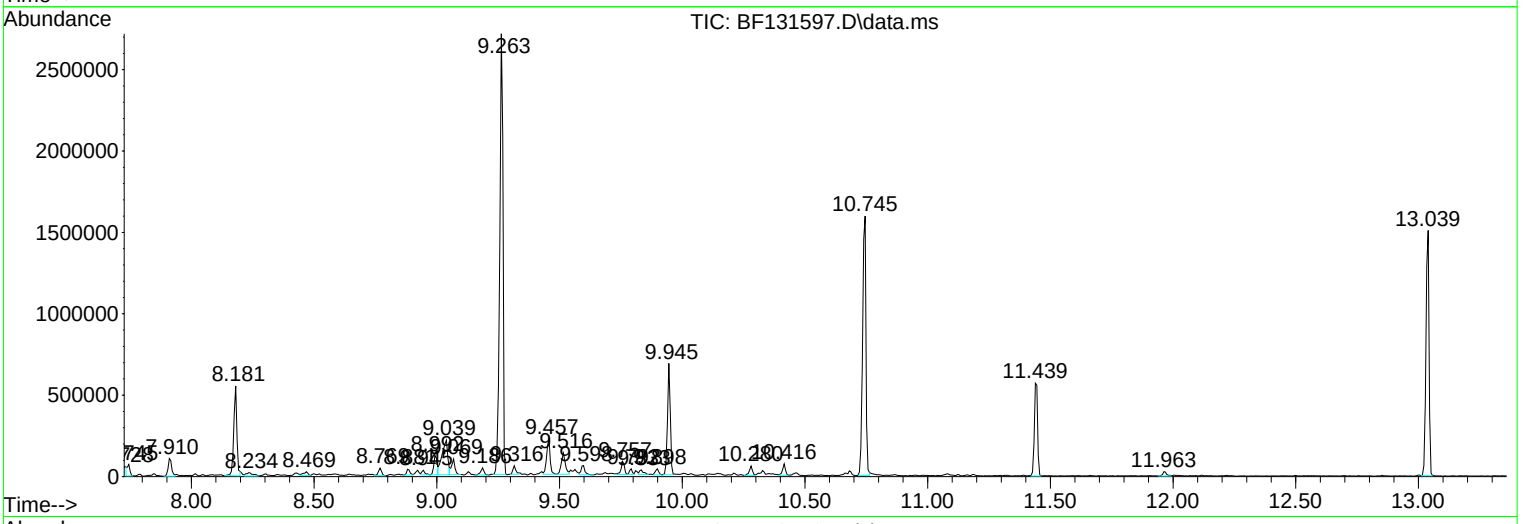
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

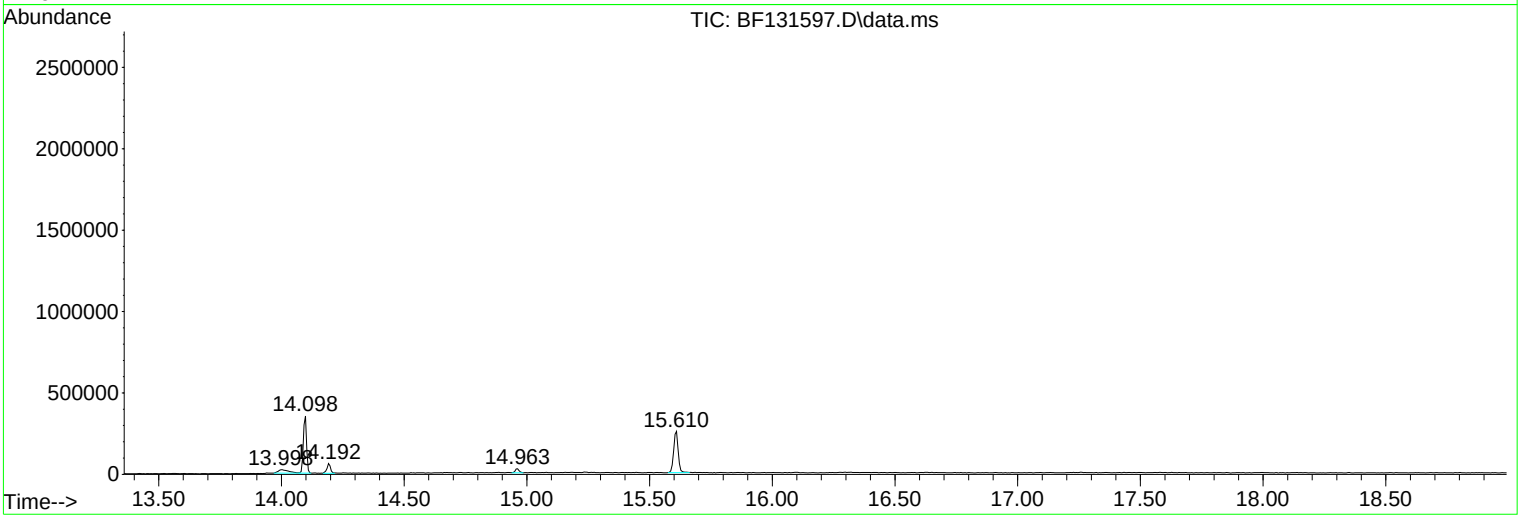
Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

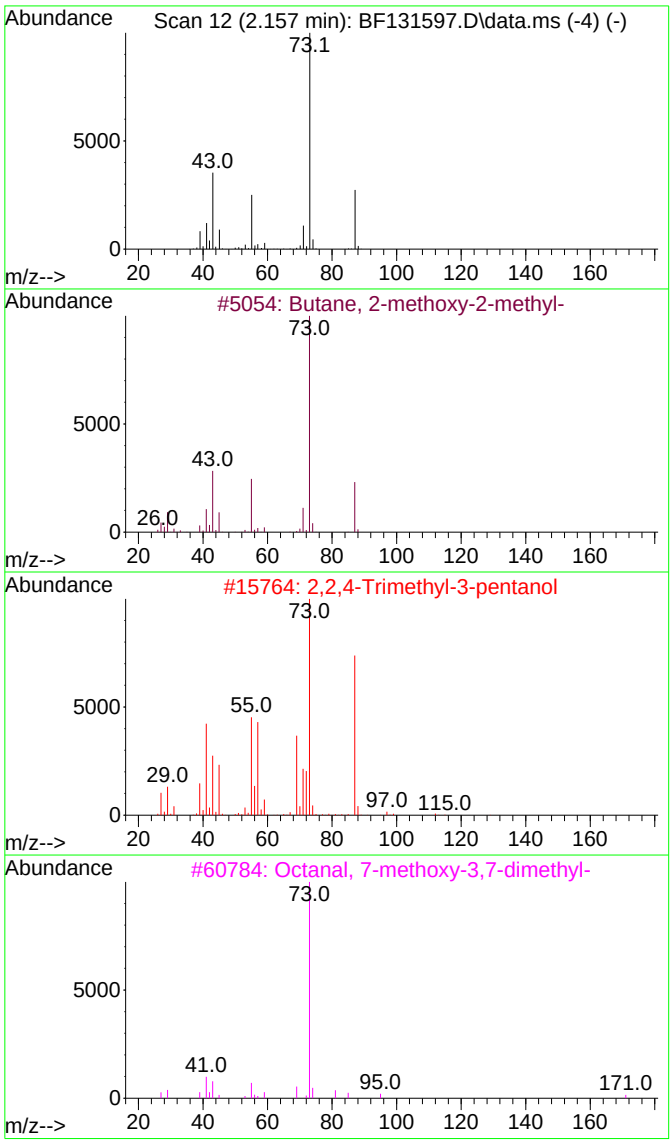
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

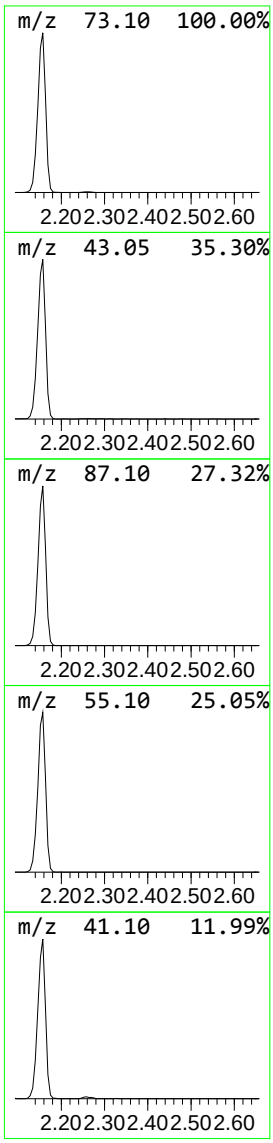
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	110.87 ng	2053080	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

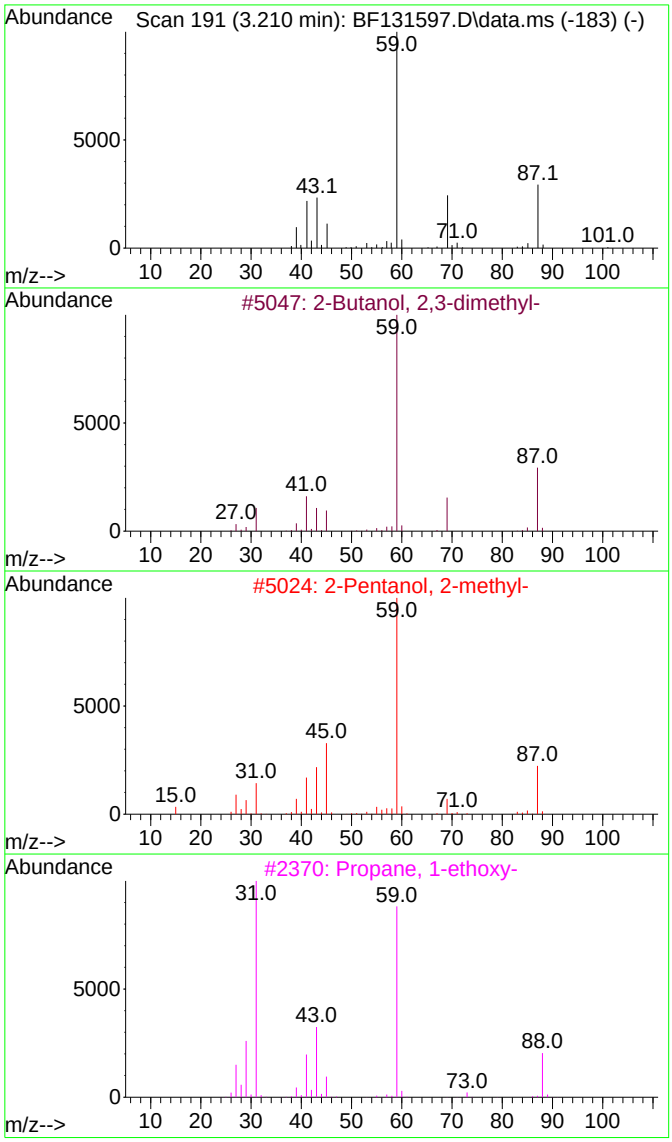
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

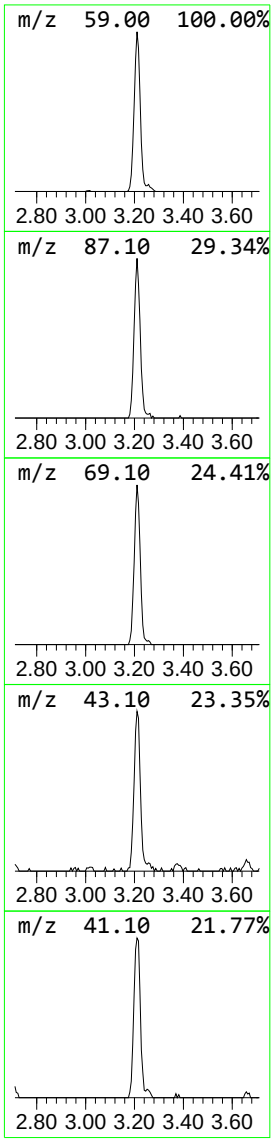
****

Peak Number 2 2-Butanol, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.210	10.89 ng	201607	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	64
3	Propane, 1-ethoxy-	88	C5H12O	000628-32-0	59
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	56
5	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

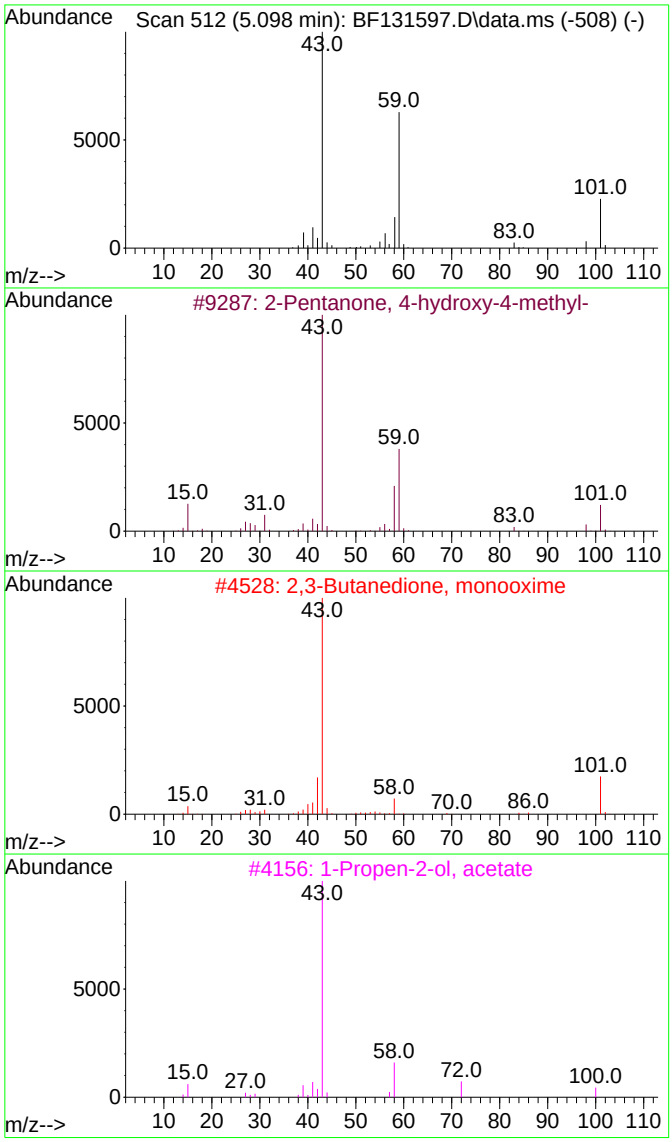
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

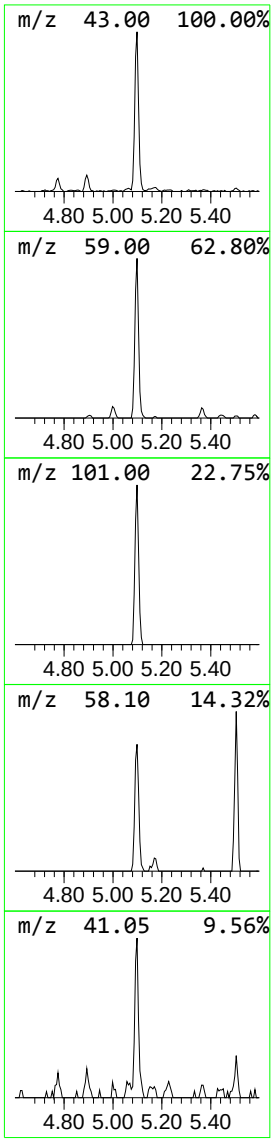
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	6.31 ng	116821	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

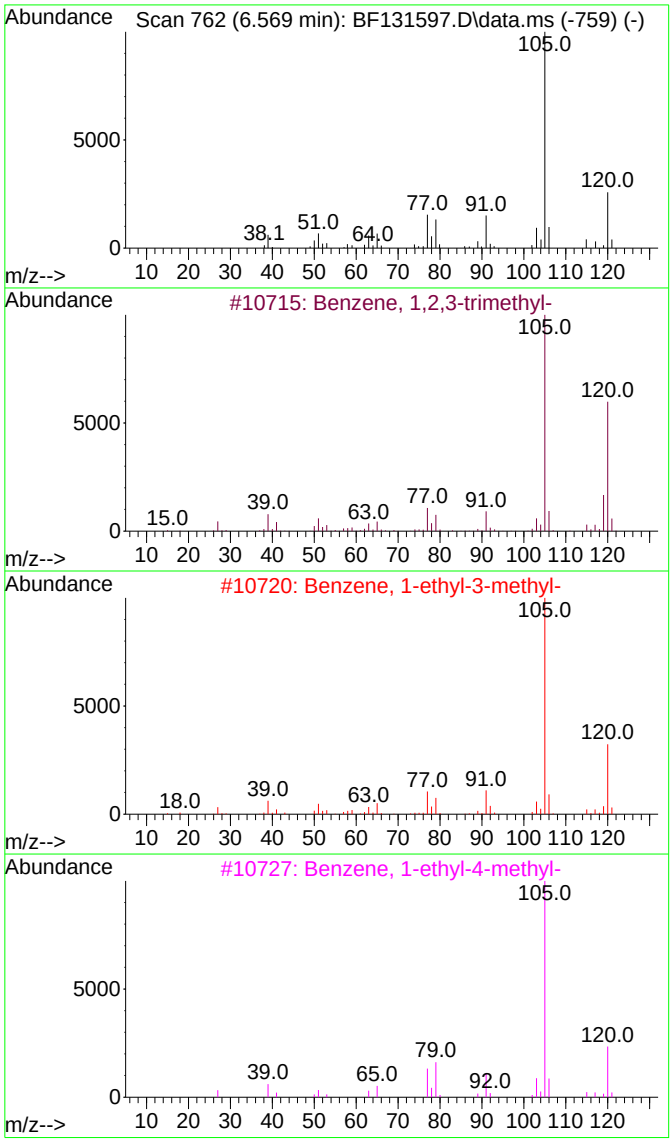
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

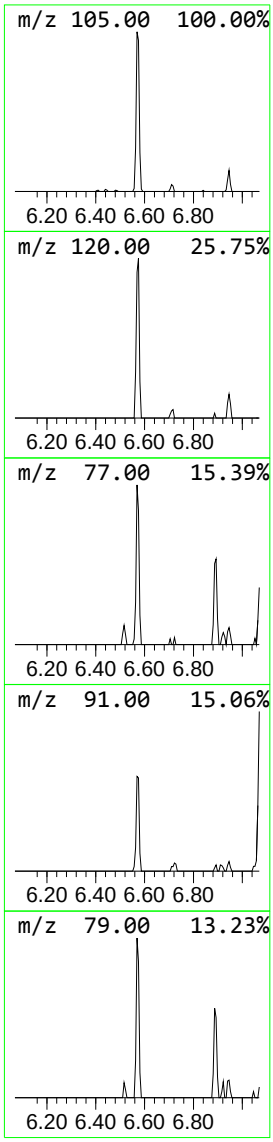
****

Peak Number 4 Benzene, 1,2,3-trimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.569	3.72 ng	68869	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
5	Mesitylene	120	C9H12	000108-67-8	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

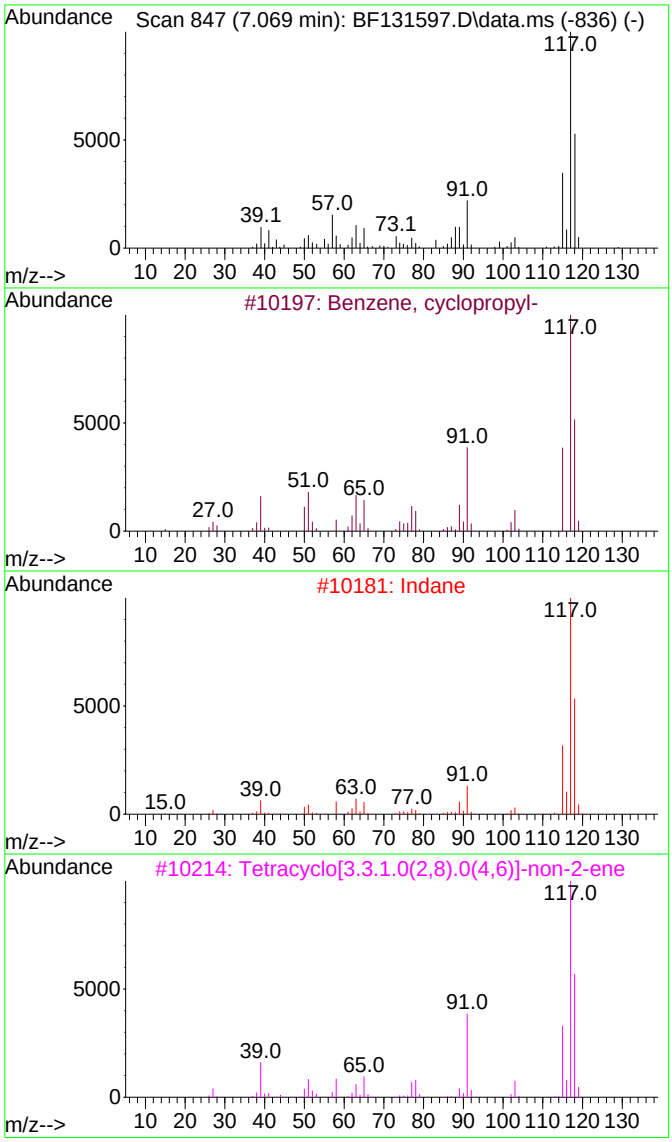
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

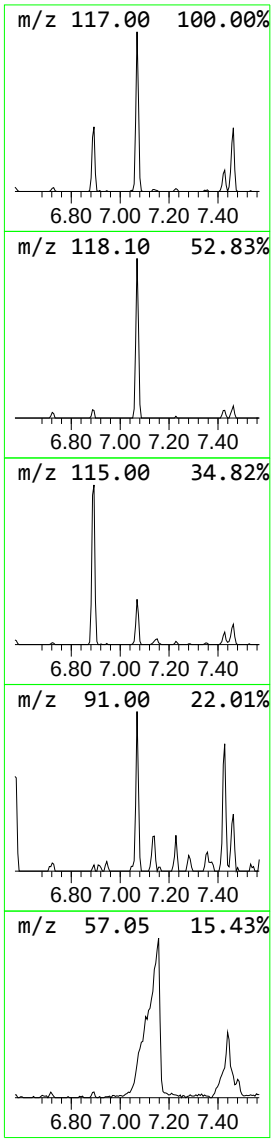
****

Peak Number 5 Benzene, cyclopropyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.069	8.80 ng	162982	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
2	Indane	118	C9H10	000496-11-7	76
3	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	76
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	50
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

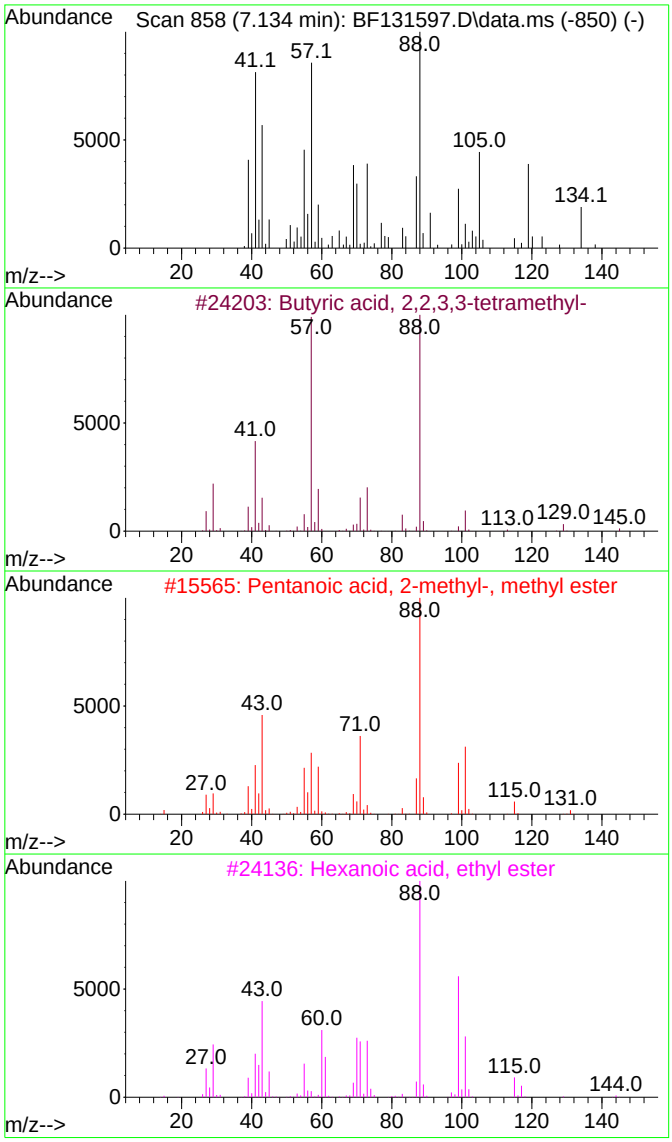
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

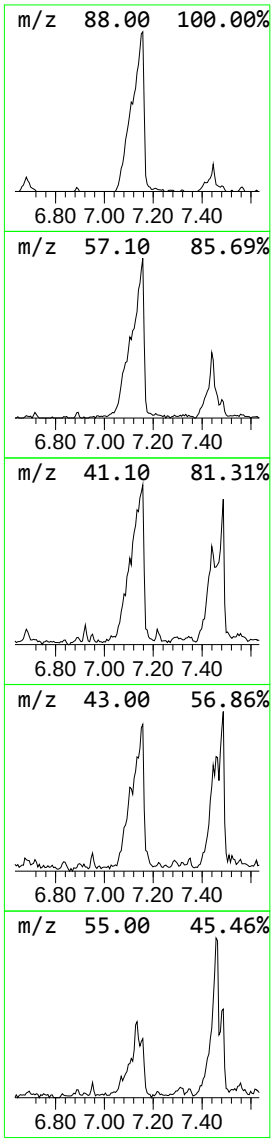
****

Peak Number 6 unknown7.134 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.134	19.72 ng	365189	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	43
2	Pentanoic acid, 2-methyl-, methy...	130	C7H14O2	002177-77-7	38
3	Hexanoic acid, ethyl ester	144	C8H16O2	000123-66-0	38
4	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	38
5	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

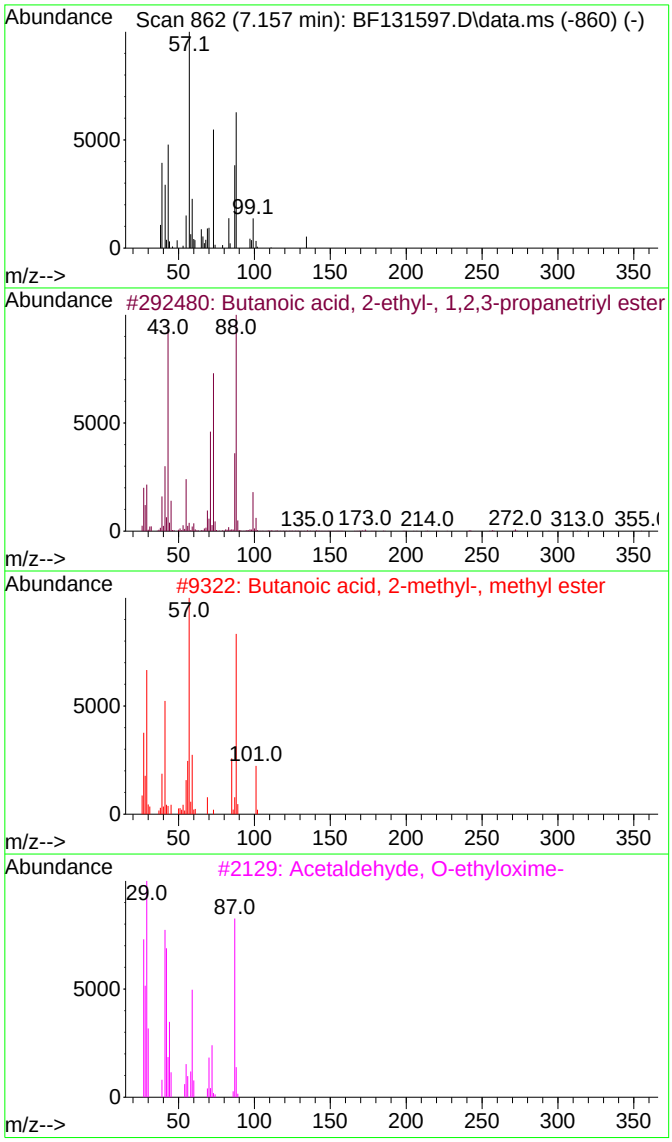
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

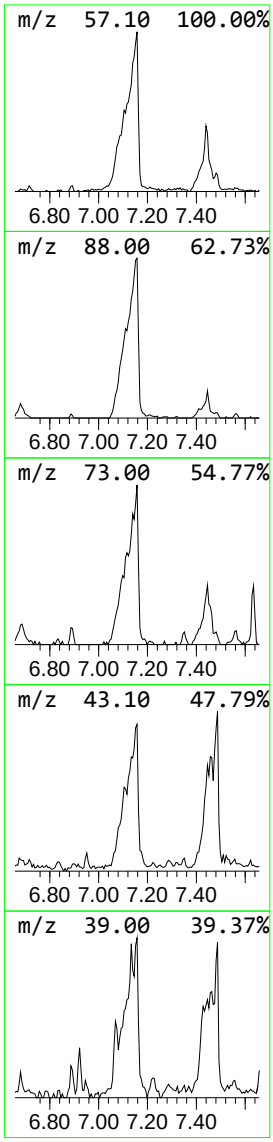
****

Peak Number 7 unknown7.157 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.157	8.06 ng	149182	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	22
2	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	17
3	Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	14
4	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	12
5	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

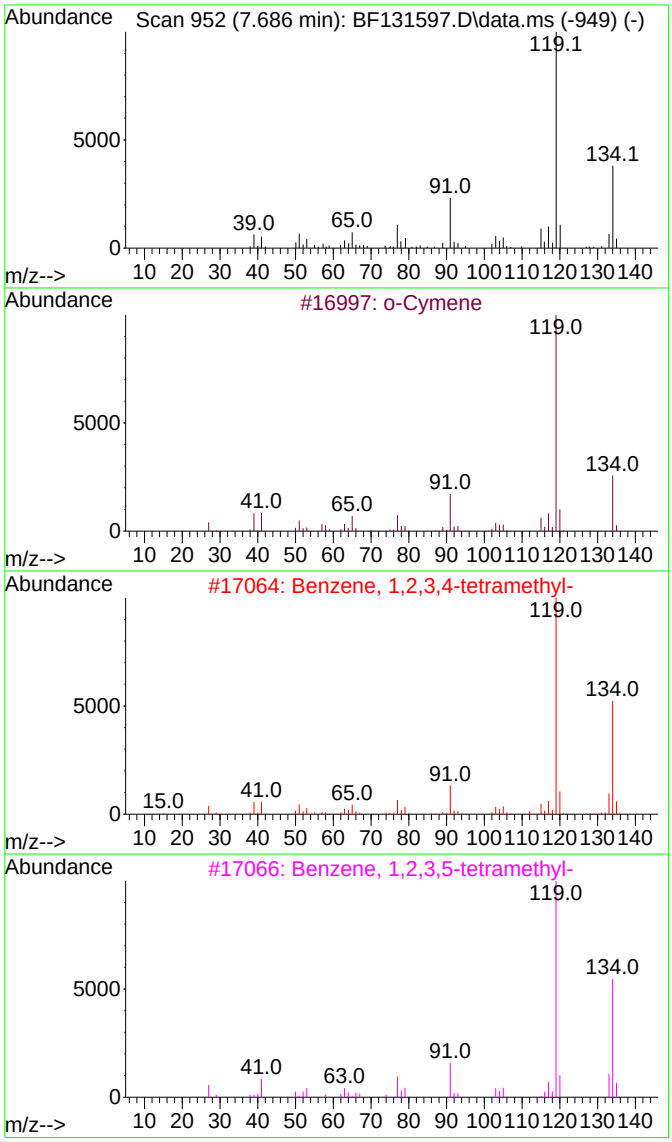
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

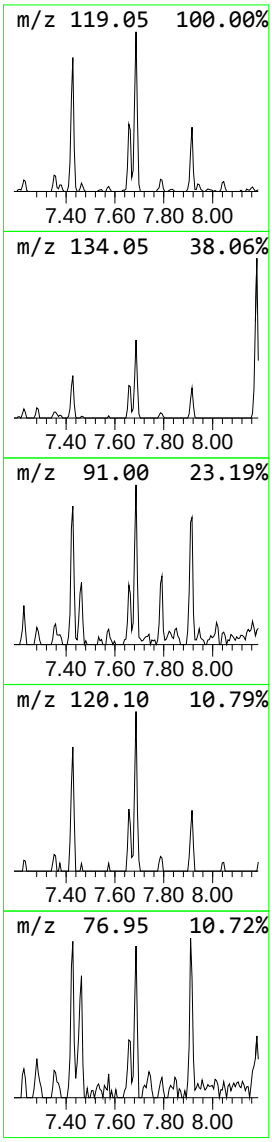
****

Peak Number 8 o-Cymene Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.686	2.86 ng	69470	Naphthalene-d8	8.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	97
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

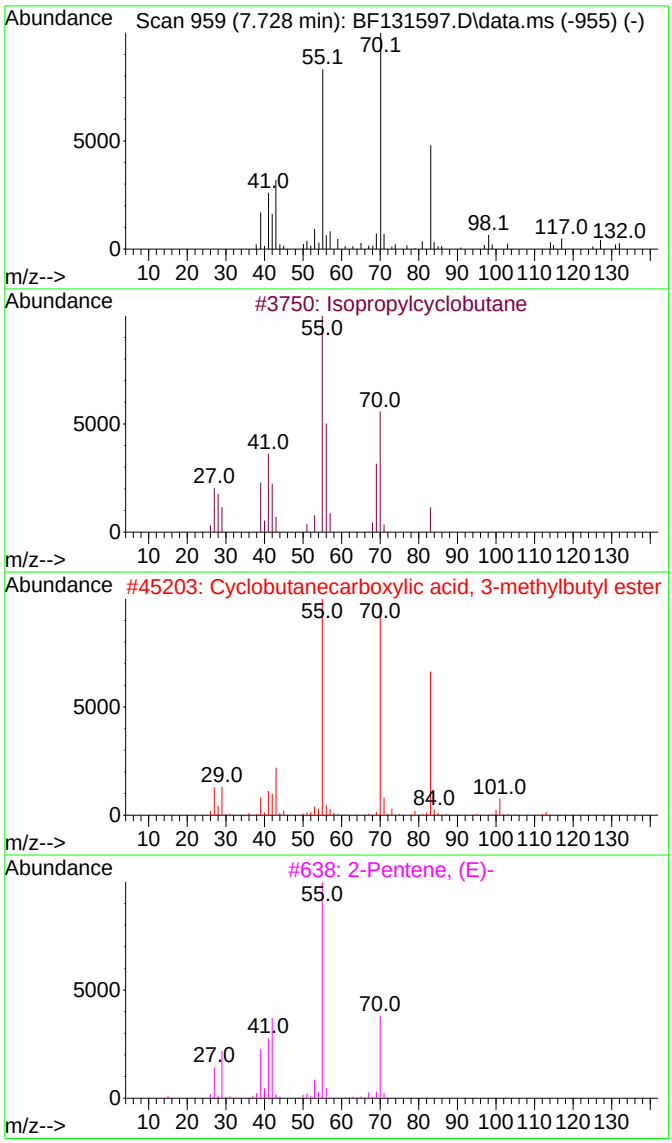
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

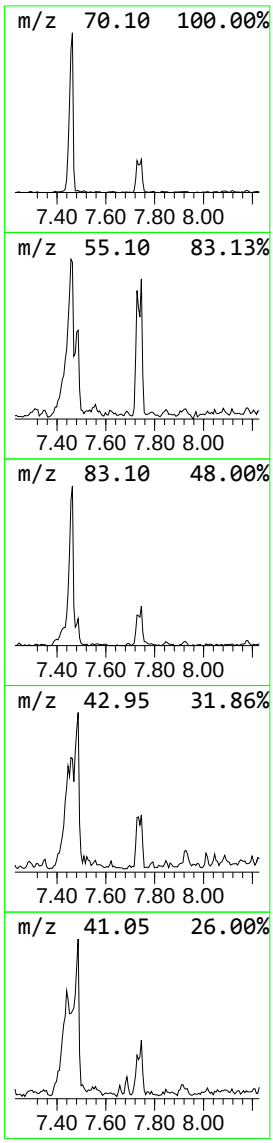
****

Peak Number 9 Isopropylcyclobutane Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.728	2.21 ng	53641	Naphthalene-d8	8.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropylcyclobutane	98	C7H14	000872-56-0	72
2	Cyclobutanecarboxylic acid, 3-me...	170	C10H18O2	1000282-21-7	64
3	2-Pentene, (E)-	70	C5H10	000646-04-8	52
4	2-Pentene	70	C5H10	000109-68-2	52
5	2-Methyl-1-butene	70	C5H10	000563-46-2	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

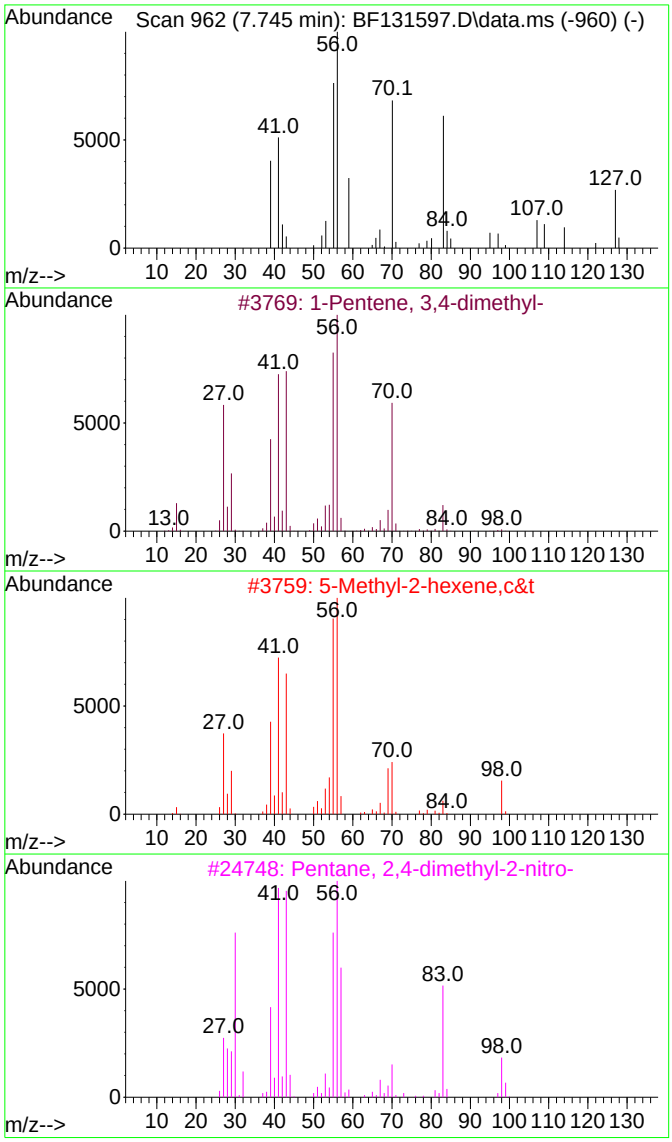
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

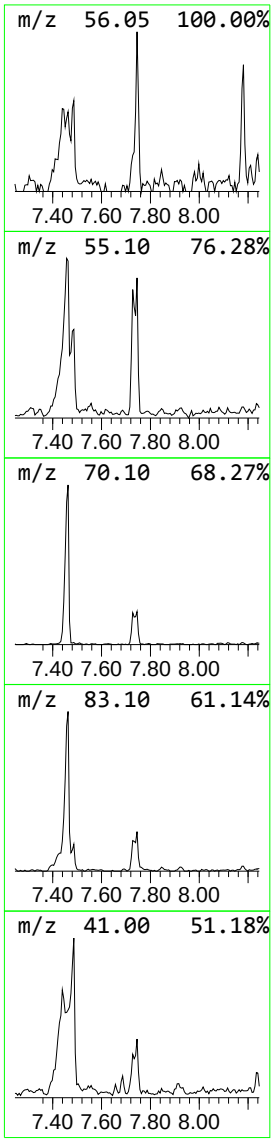
****

Peak Number 10 1-Pentene, 3,4-dimethyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.745	2.16 ng	52469	Naphthalene-d8	8.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 3,4-dimethyl-	98	C7H14	007385-78-6	50
2	5-Methyl-2-hexene,c&t	98	C7H14	003404-62-4	43
3	Pentane, 2,4-dimethyl-2-nitro-	145	C7H15NO2	000597-45-5	40
4	Formic acid, octyl ester	158	C9H18O2	000112-32-3	38
5	2-Hexene, 5-methyl-, (E)-	98	C7H14	007385-82-2	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

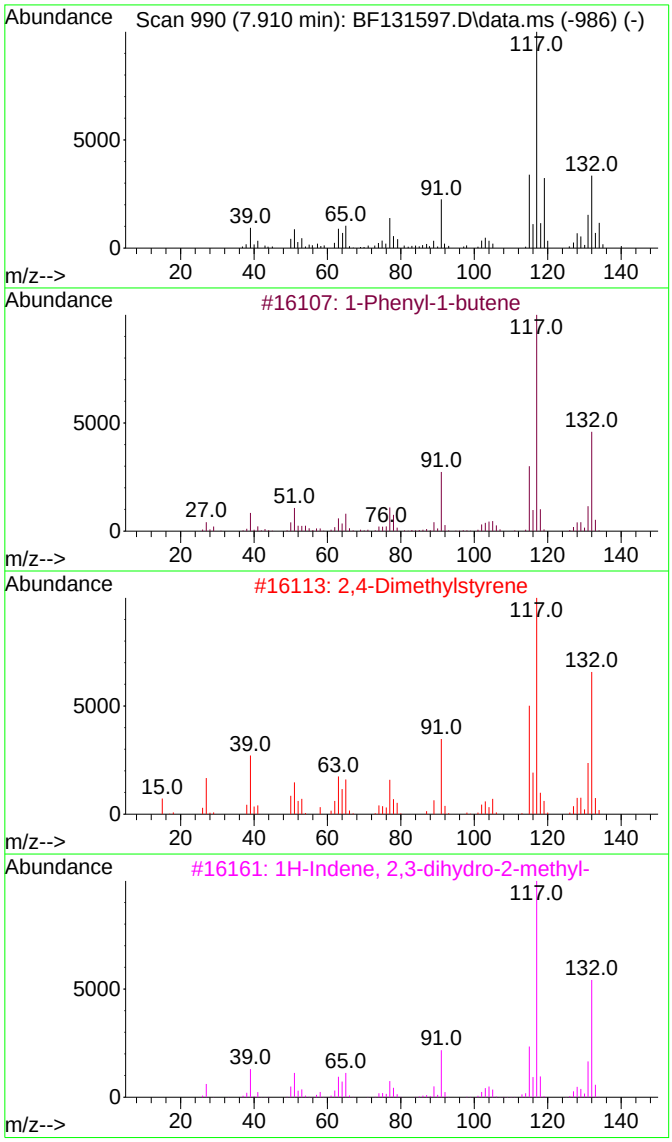
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

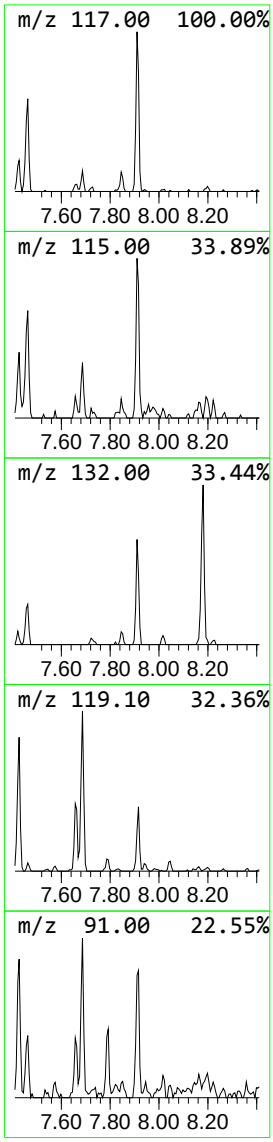
****

Peak Number 11 1-Phenyl-1-butene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.910	4.49 ng	109139	Naphthalene-d8	8.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-butene	132	C10H12	000824-90-8	94
2	2,4-Dimethylstyrene	132	C10H12	002234-20-0	92
3	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	91
4	(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	91
5	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

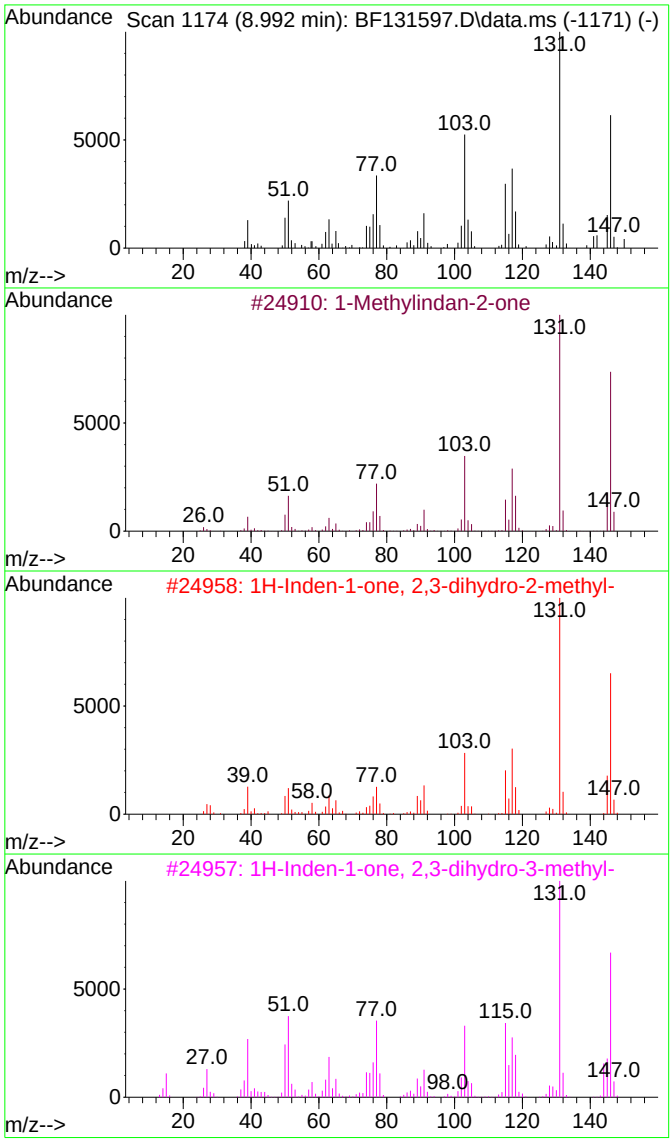
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

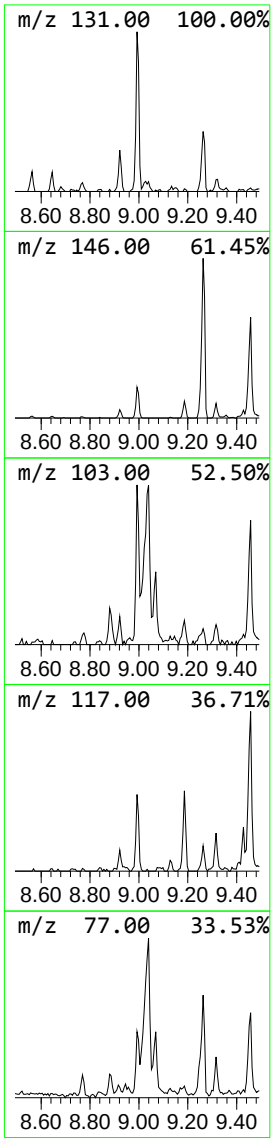
****

Peak Number 12 1-Methylindan-2-one Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.992	4.67 ng	113595	Naphthalene-d8	8.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methylindan-2-one	146	C10H10O	035587-60-1	95
2	1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	91
3	1H-Inden-1-one, 2,3-dihydro-3-me...	146	C10H10O	006072-57-7	91
4	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	70
5	3-Buten-2-one, 4-phenyl-, (E)-	146	C10H10O	001896-62-4	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

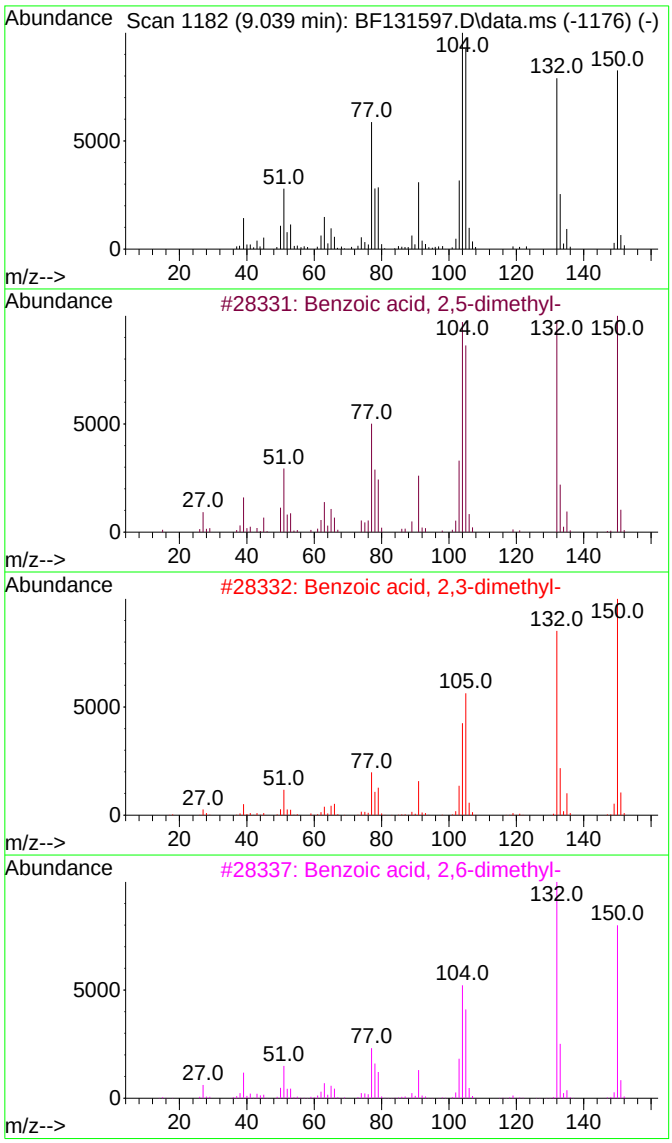
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

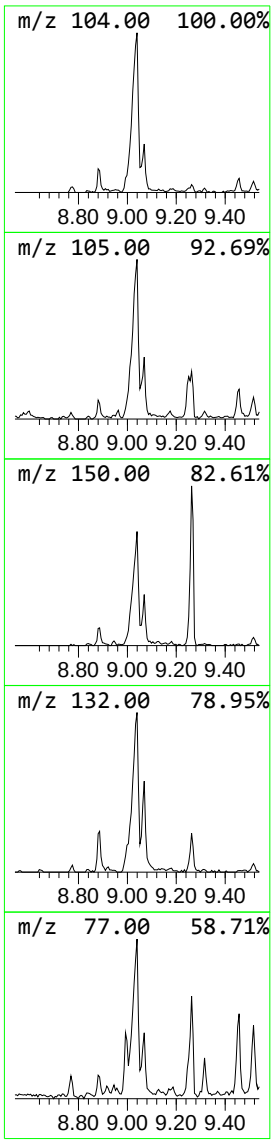
****

Peak Number 13 Benzoic acid, 2,5-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.039	14.18 ng	344727	Naphthalene-d8	8.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,5-dimethyl-	150	C9H10O2	000610-72-0	97
2	Benzoic acid, 2,3-dimethyl-	150	C9H10O2	000603-79-2	83
3	Benzoic acid, 2,6-dimethyl-	150	C9H10O2	000632-46-2	76
4	para-Methylbenzyl formate	150	C9H10O2	1000368-93-7	64
5	Formic acid, 1-phenylethyl ester	150	C9H10O2	1000368-94-1	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

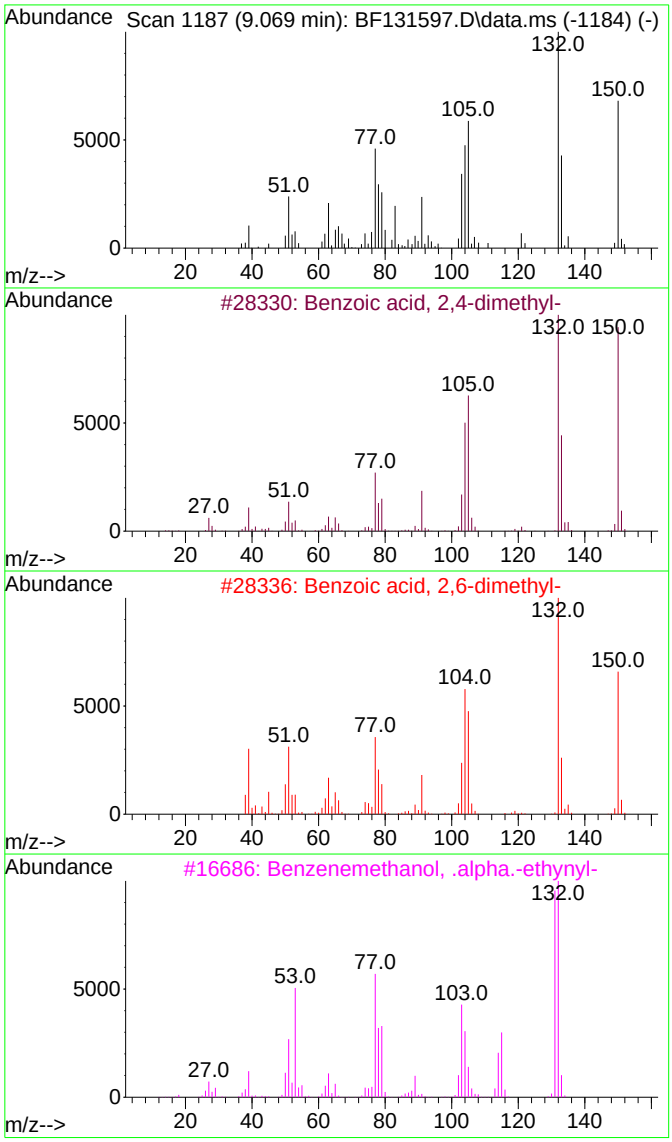
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

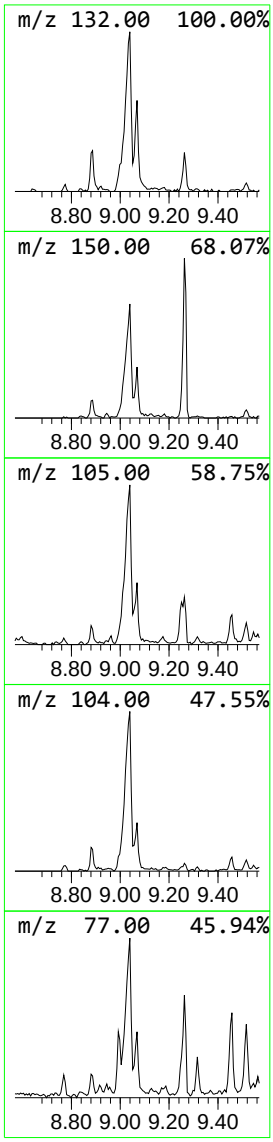
****

Peak Number 14 Benzoic acid, 2,4-dimethyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.069	3.38 ng	90676	Acenaphthene-d10	9.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,4-dimethyl-	150	C9H10O2	000611-01-8	64
2	Benzoic acid, 2,6-dimethyl-	150	C9H10O2	000632-46-2	58
3	Benzenemethanol, .alpha.-ethynyl-	132	C9H8O	004187-87-5	49
4	Benzoic acid, 2,5-dimethyl-	150	C9H10O2	000610-72-0	46
5	Isoquinoline, 1,2,3,4-tetrahydro-	133	C9H11N	000091-21-4	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

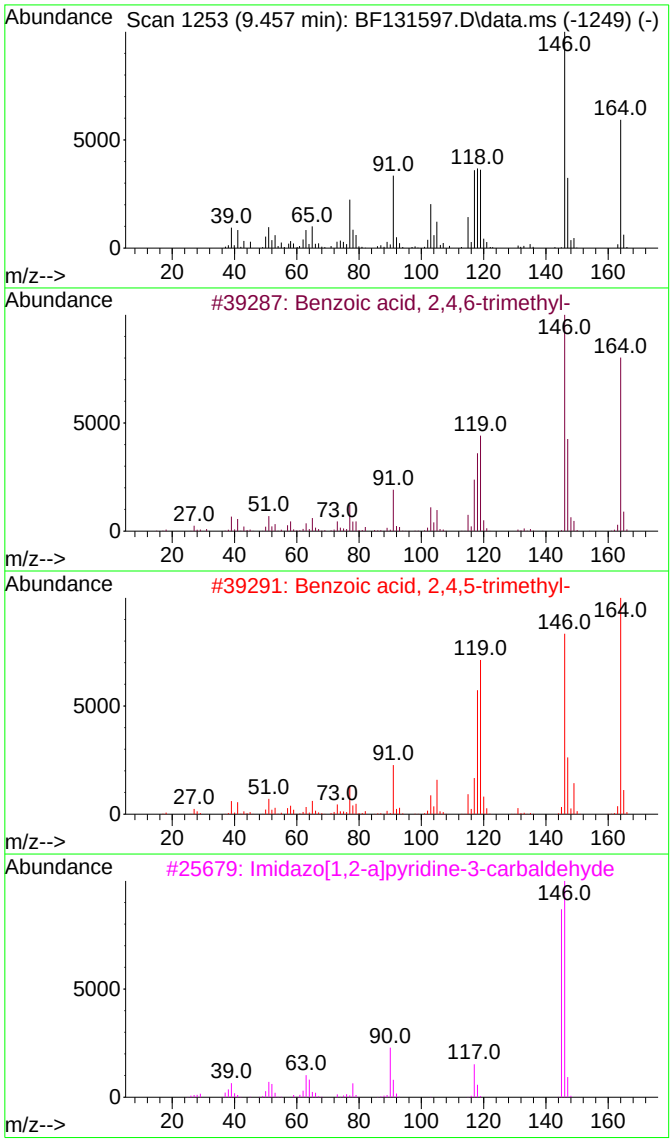
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

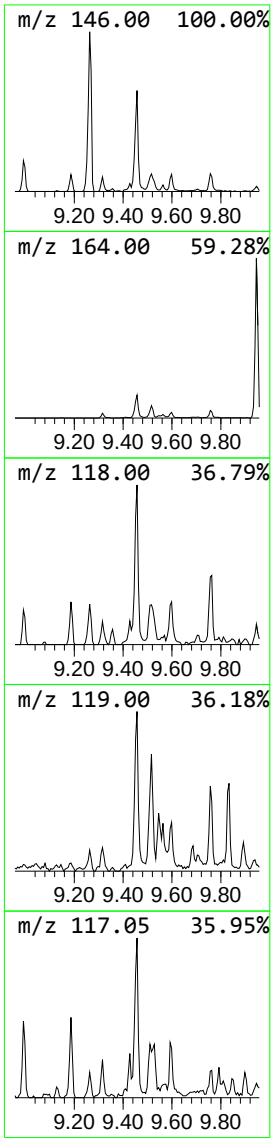
****

Peak Number 15 Benzoic acid, 2,4,6-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.457	7.77 ng	208150	Acenaphthene-d10	9.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,4,6-trimethyl-	164	C10H12O2	000480-63-7	90
2	Benzoic acid, 2,4,5-trimethyl-	164	C10H12O2	000528-90-5	47
3	Imidazo[1,2-a]pyridine-3-carbald...	146	C8H6N2O	006188-43-8	35
4	2-Propenamide, 3-phenyl-	147	C9H9NO	000621-79-4	35
5	3-Bromo-1H-pyrazole	146	C3H3BrN2	014521-80-3	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

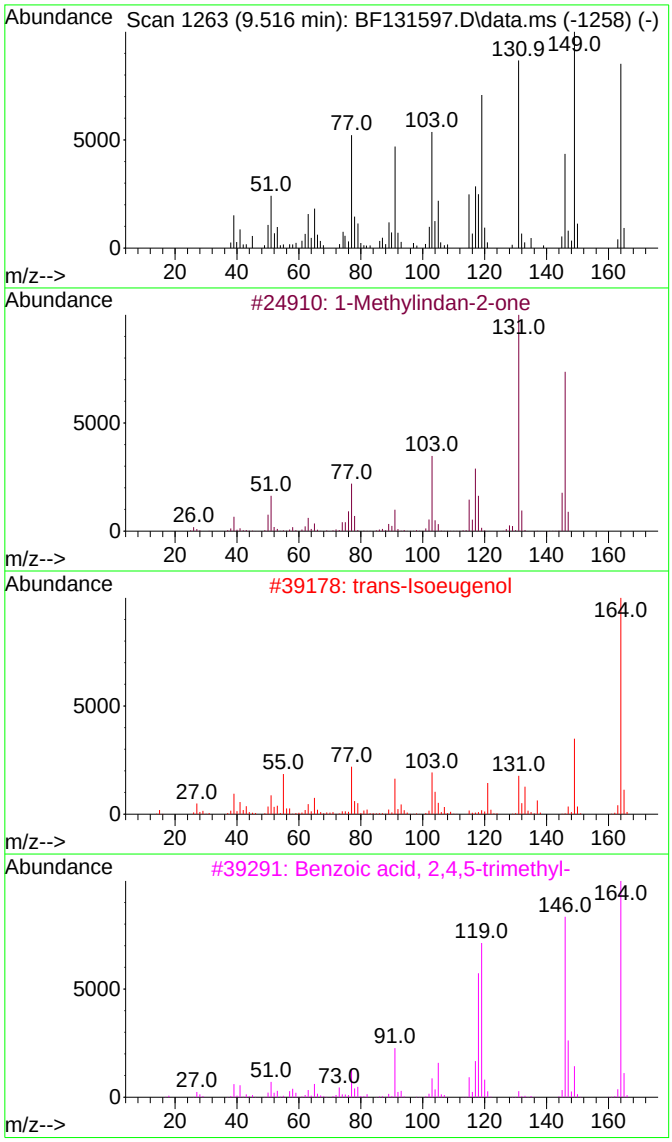
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

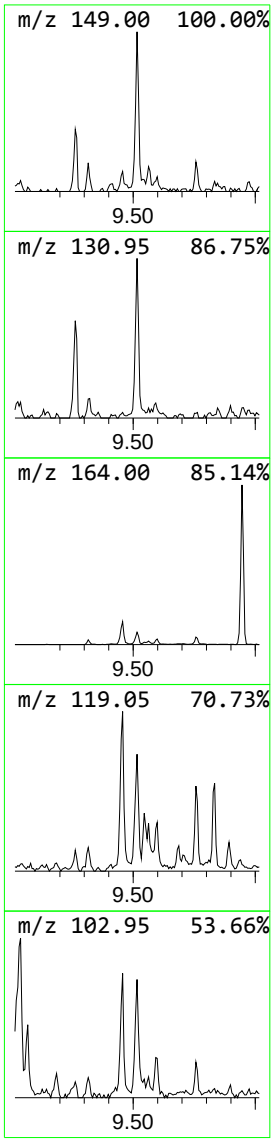
****

Peak Number 16 unknown9.516 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.516	5.58 ng	149579	Acenaphthene-d10	9.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methylindan-2-one	146	C10H10O	035587-60-1	50
2	trans-Isoeugenol	164	C10H12O2	005932-68-3	46
3	Benzoic acid, 2,4,5-trimethyl-	164	C10H12O2	000528-90-5	43
4	1,3-Benzenediamine, N,N'-diethyl-	164	C10H16N2	005857-99-8	38
5	2,3,4,5,6-Pentamethylphenol	164	C11H16O	002819-86-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

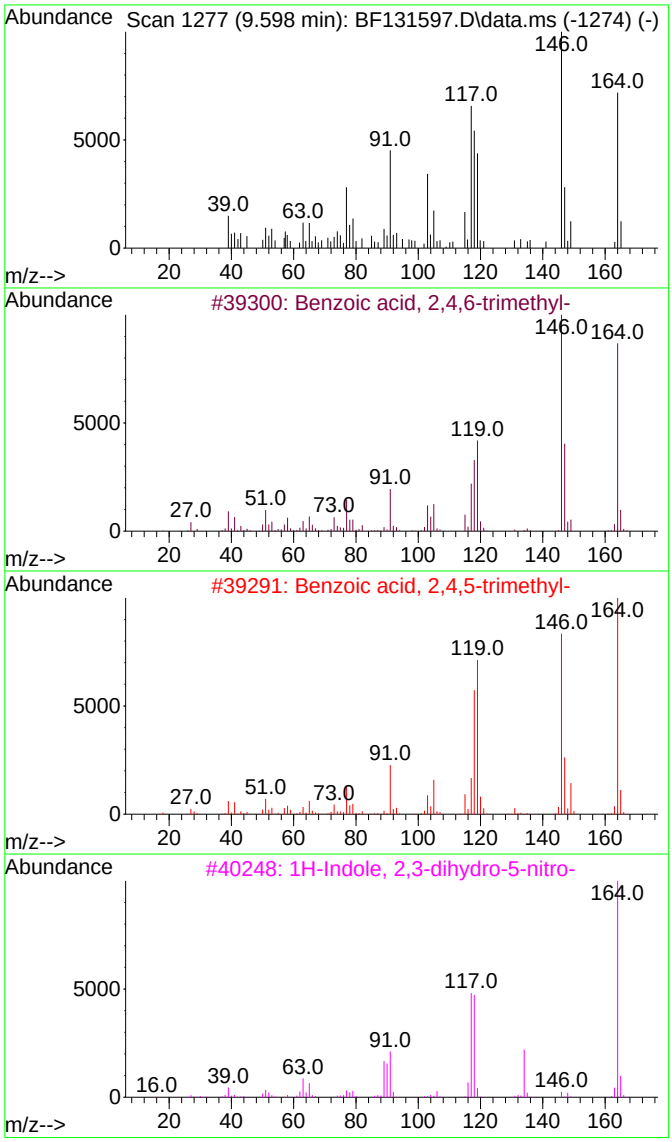
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

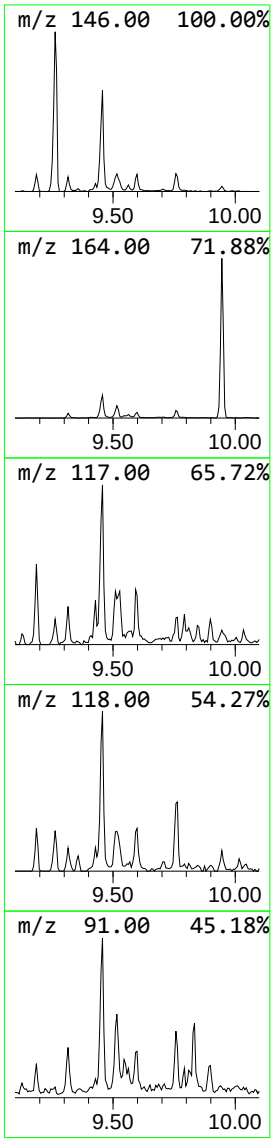
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 Benzoic acid, 2,4,5-trimethyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.598	2.29 ng	61473	Acenaphthene-d10	9.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,4,6-trimethyl-	164	C10H12O2	000480-63-7	76
2	Benzoic acid, 2,4,5-trimethyl-	164	C10H12O2	000528-90-5	58
3	1H-Indole, 2,3-dihydro-5-nitro-	164	C8H8N2O2	032692-19-6	38
4	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	35
5	p-Coumaric acid	164	C9H8O3	007400-08-0	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

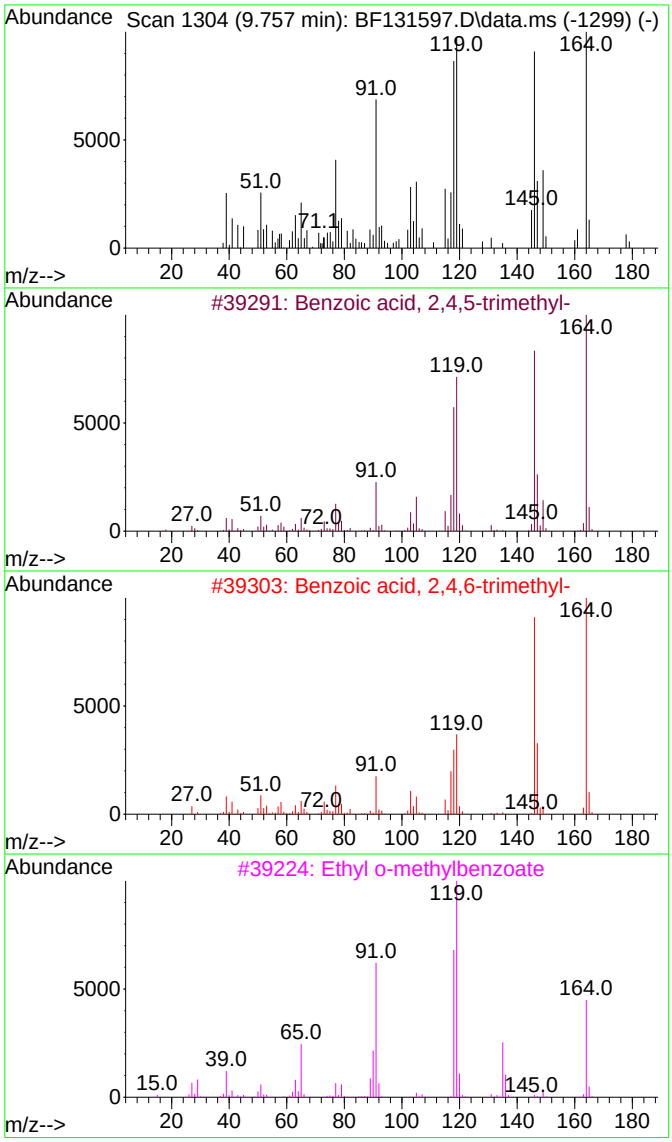
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

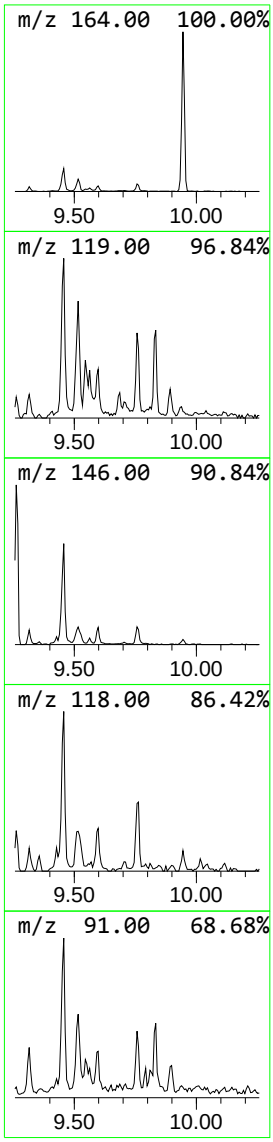
****

Peak Number 18 unknown9.757 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.757	2.81 ng	75332	Acenaphthene-d10	9.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,4,5-trimethyl-	164	C10H12O2	000528-90-5	95
2	Benzoic acid, 2,4,6-trimethyl-	164	C10H12O2	000480-63-7	49
3	Ethyl o-methylbenzoate	164	C10H12O2	000087-24-1	46
4	1-Propanamine, N-(phenylmethylene)-	147	C10H13N	006852-55-7	46
5	3,5-Dimethylphenylacetic acid	164	C10H12O2	042288-46-0	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

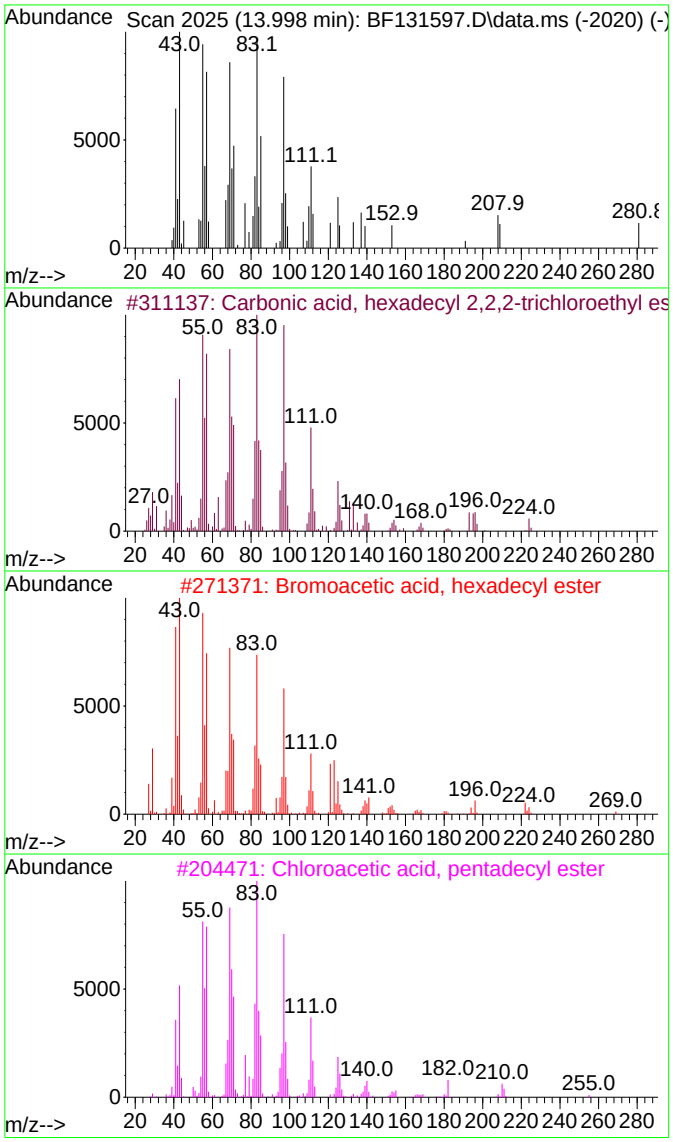
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

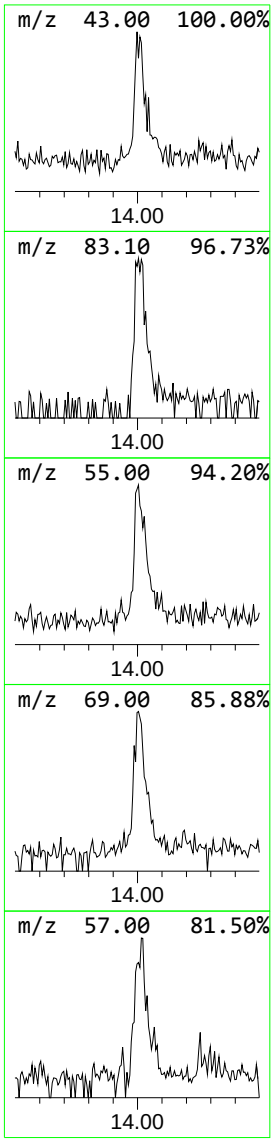
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 Carbonic acid, hexadecyl 2,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	4.03 ng	63914	Chrysene-d12	14.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	87
2	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	81
3	Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	74
4	1-Heptadecene	238	C17H34	006765-39-5	74
5	1-Hexacosene	364	C26H52	018835-33-1	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

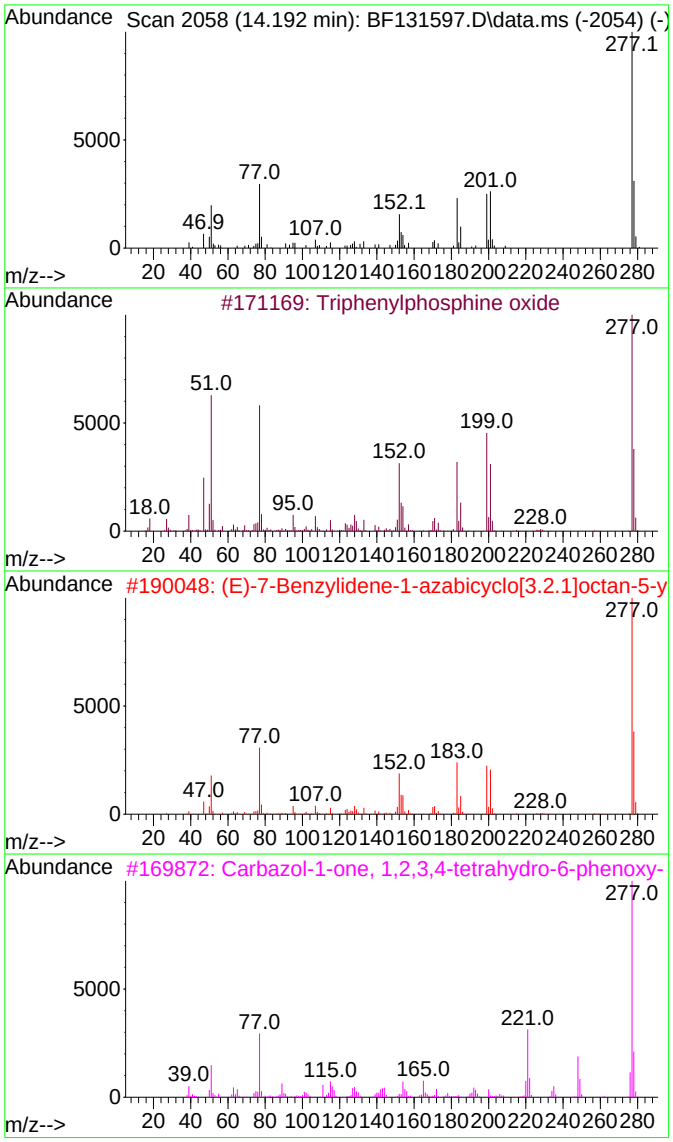
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

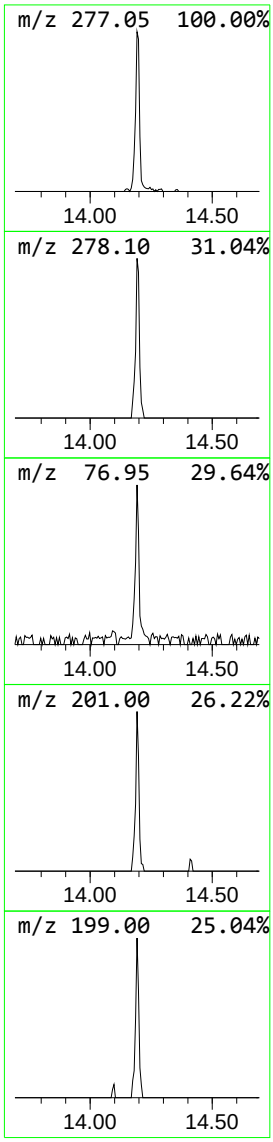
****

Peak Number 20 Triphenylphosphine oxide Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.192	3.83 ng	60800	Chrysene-d12	14.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	83
3	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	43
4	Furo[3,2-c]quinoline, 8-bromo-2,...	277	C13H12BrNO	1000310-92-7	32
5	3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131597.D
Acq On : 12 Dec 2022 17:35
Operator : CG\JU
Sample : N6001-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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...	2.157	110.9	ng	2053080	1	6.892	370354	20.0
2-Butanol, 2,3-...	3.210	10.9	ng	201607	1	6.892	370354	20.0
2-Pentanone, 4-...	5.098	6.3	ng	116821	1	6.892	370354	20.0
Benzene, 1,2,3-...	6.569	3.7	ng	68869	1	6.892	370354	20.0
Benzene, cyclop...	7.069	8.8	ng	162982	1	6.892	370354	20.0
unknown7.134	7.134	19.7	ng	365189	1	6.892	370354	20.0
unknown7.157	7.157	8.1	ng	149182	1	6.892	370354	20.0
o-Cymene	7.686	2.9	ng	69470	2	8.181	486382	20.0
Isopropylcyclob...	7.728	2.2	ng	53641	2	8.181	486382	20.0
1-Pentene, 3,4-...	7.745	2.2	ng	52469	2	8.181	486382	20.0
1-Phenyl-1-butene	7.910	4.5	ng	109139	2	8.181	486382	20.0
1-Methylindan-2...	8.992	4.7	ng	113595	2	8.181	486382	20.0
Benzoic acid, 2...	9.039	14.2	ng	344727	2	8.181	486382	20.0
Benzoic acid, 2...	9.069	3.4	ng	90676	3	9.945	535940	20.0
Benzoic acid, 2...	9.457	7.8	ng	208150	3	9.945	535940	20.0
unknown9.516	9.516	5.6	ng	149579	3	9.945	535940	20.0
Benzoic acid, 2...	9.598	2.3	ng	61473	3	9.945	535940	20.0
unknown9.757	9.757	2.8	ng	75332	3	9.945	535940	20.0
Carbonic acid, ...	13.998	4.0	ng	63914	5	14.098	317225	20.0
Triphenylphosph...	14.192	3.8	ng	60800	5	14.098	317225	20.0