LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129810.D
Acq On : 16 Aug 2022 14:19
Operator : CG\JU
Sample : N3971-24
Misc :
ALS Vial : 11 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : COP-1R

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-BF081422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129810.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.881	267	271	282	rVB	442322	611713	10.86%	1.333%
2	4.328	343	347	360	rBV	747857	933324	16.58%	2.034%
3	5.046	466	469	492	rBV	509857	615753	10.94%	1.342%
4	5.299	509	512	520	rVB	197961	179529	3.19%	0.391%
5	5.404	527	530	532	rBV	431643	393967	7.00%	0.859%
6	5.463	537	540	557	rVB	2691923	2616358	46.47%	5.702%
7	5.622	564	567	571	rBV	81638	74090	1.32%	0.161%
8	5.663	571	574	579	rVB	459390	432423	7.68%	0.942%
9	6.122	649	652	670	rBV	540261	515225	9.15%	1.123%
10	6.340	686	689	692	rBV	79304	63337	1.12%	0.138%
11	6.475	708	712	726	rBV	1983237	1977174	35.11%	4.309%
12	6.640	736	740	748	rBV	158448	161967	2.88%	0.353%
13	6.822	767	771	774	rBV	2172812	1917365	34.05%	4.179%
14	6.881	774	781	793	rVV2	188301	289535	5.14%	0.631%
15	6.993	794	800	804	rVB2	56206	109219	1.94%	0.238%
16	7.228	834	840	845	rBV2	108996	138560	2.46%	0.302%
17	7.393	858	868	871	rBV	2804355	2953420	52.45%	6.437%
18	7.463	877	880	885	rBV	51830	79959	1.42%	0.174%
19	7.510	885	888	900	rVB2	51993	97968	1.74%	0.214%
20	7.640	903	910	917	rBV	256049	248042	4.41%	0.541%
21	8.016	970	974	980	rBV3	98885	204600	3.63%	0.446%
22	8.104	985	989	992	rBV	3022682	2700884	47.97%	5.886%
23	8.275	1015	1018	1025	rBV	65829	135322	2.40%	0.295%
24	8.428	1040	1044	1049	rBV2	50897	90358	1.60%	0.197%
25	8.534	1056	1062	1069	rVB	512468	748626	13.30%	1.632%
26	8.757	1097	1100	1106	rVB	75227	74277	1.32%	0.162%
27	8.810	1106	1109	1112	rBV2	64856	61985	1.10%	0.135%
28	9.069	1148	1153	1156	rBV	78659	141969	2.52%	0.309%
29	9.098	1156	1158	1164	rVB	62520	75997	1.35%	0.166%
30	9.181	1165	1172	1175	rBV	5987633	5630712	100.00%	12.271%
31	9.287	1186	1190	1204	rVB	2306480	2066092	36.69%	4.503%
32	9.604	1242	1244	1253	rVB5	68833	93259	1.66%	0.203%
33	9.822	1276	1281	1283	rBV	73693	72306	1.28%	0.158%
34	9.863	1283	1288	1291	rBV	3701151	3090100	54.88%	6.734%
35	10.169	1335	1340	1343	rBV2	55268	69328	1.23%	0.151%
36	10.275	1355	1358	1363	rVB	133190	114643	2.04%	0.250%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129810.D
Acq On : 16 Aug 2022 14:19
Operator : CG\JU
Sample : N3971-24
Misc :
ALS Vial : 11 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
COP-1R

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-BF081422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	10.563	1404	1407	1414	rVB3	113364	169234	3.01%	0.369%
38	10.657	1419	1423	1426	rBV	3612529	3059742	54.34%	6.668%
39	10.992	1476	1480	1488	rBV2	36363	91009	1.62%	0.198%
40	11.163	1505	1509	1514	rVB2	69284	73221	1.30%	0.160%
41	11.351	1537	1541	1545	rBV	3299038	3008562	53.43%	6.557%
42	11.410	1548	1551	1555	rBV3	120967	122328	2.17%	0.267%
43	11.504	1564	1567	1572	rVB	145005	119711	2.13%	0.261%
44	11.586	1576	1581	1586	rBV	160764	155765	2.77%	0.339%
45	11.728	1601	1605	1608	rBV	122788	108327	1.92%	0.236%
46	12.939	1806	1811	1814	rBV	5764250	5353123	95.07%	11.666%
47	14.004	1987	1992	1995	rBV	2026359	1941995	34.49%	4.232%
48	14.733	2112	2116	2123	rBV	174764	190156	3.38%	0.414%
49	15.474	2234	2242	2252	rBV	1328742	1712757	30.42%	3.733%

Sum of corrected areas: 45885316

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
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Operator : CG\JU
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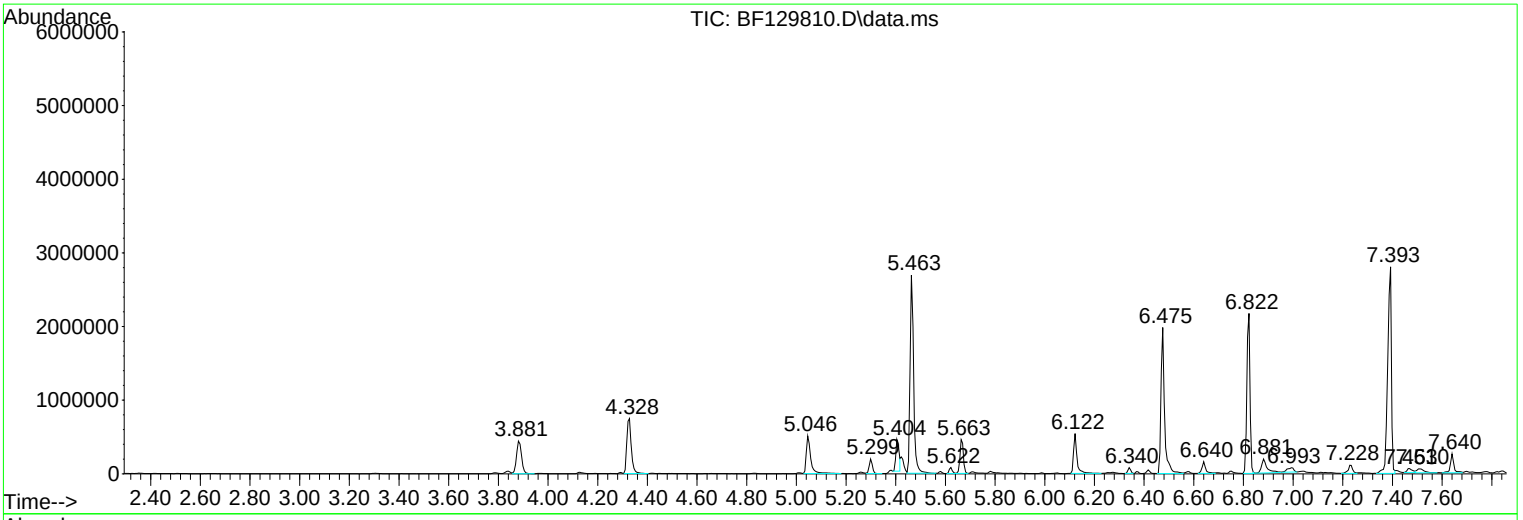
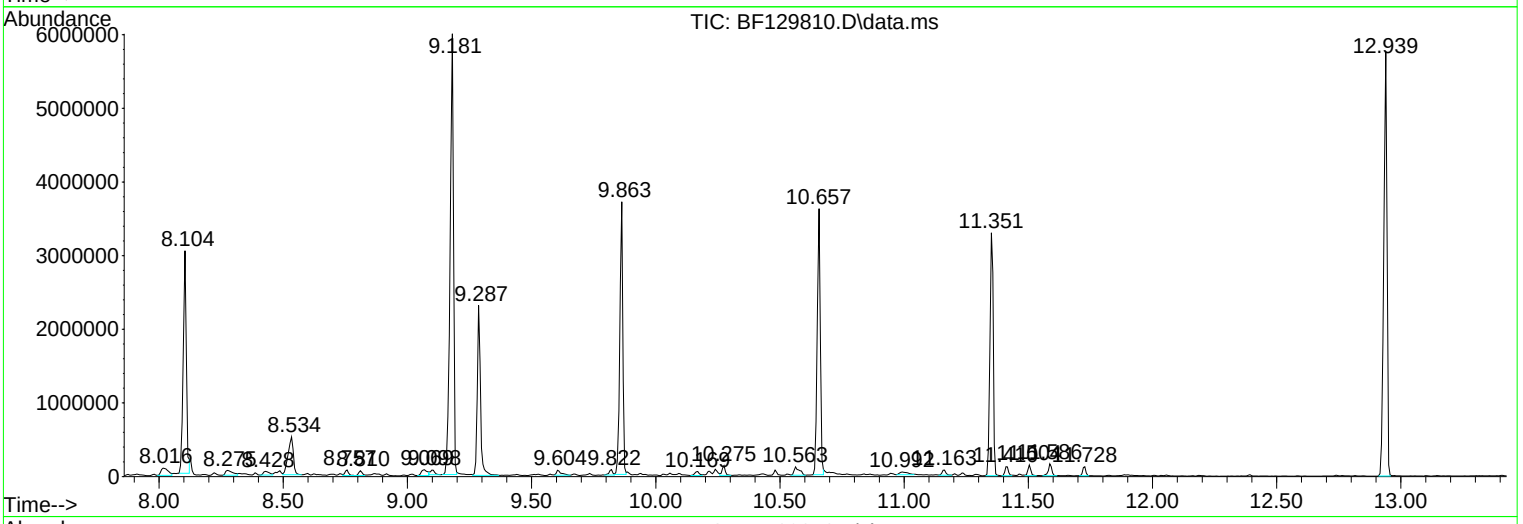
Misc :
ALS Vial : 11 Sample Multiplier: 2

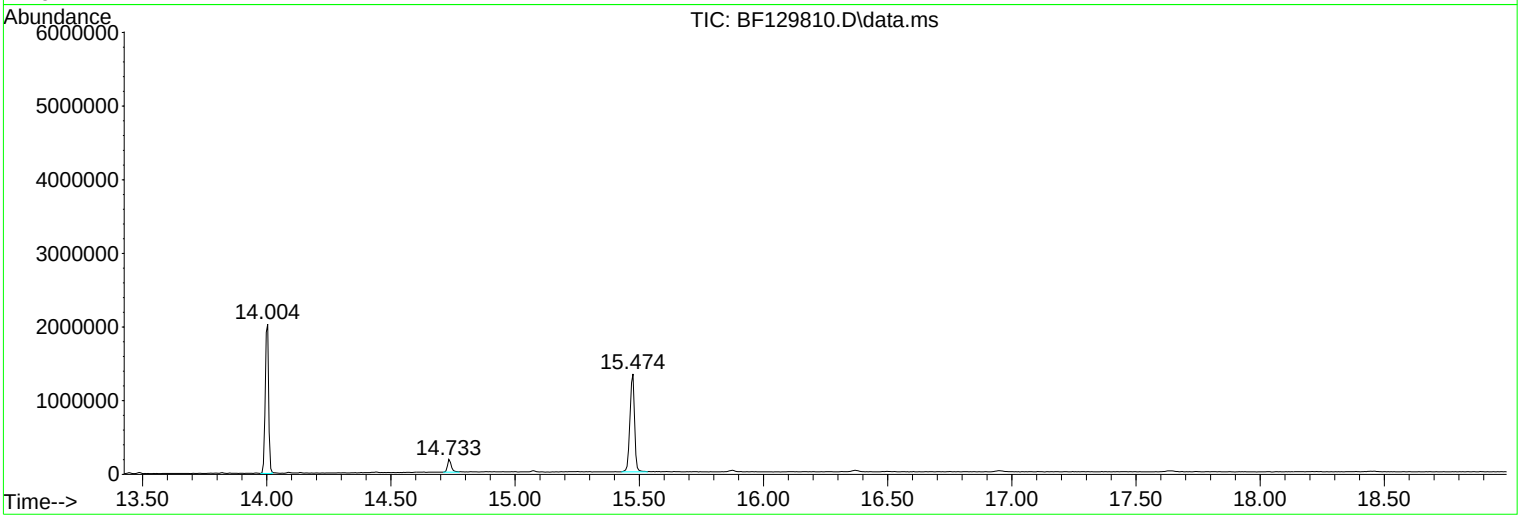
Instrument :
BNA_F
ClientSampleId :
COP-1R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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\BF081622\
Data File : BF129810.D
Acq On : 16 Aug 2022 14:19
Operator : CG\JU
Sample : N3971-24
Misc :
ALS Vial : 11 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
COP-1R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

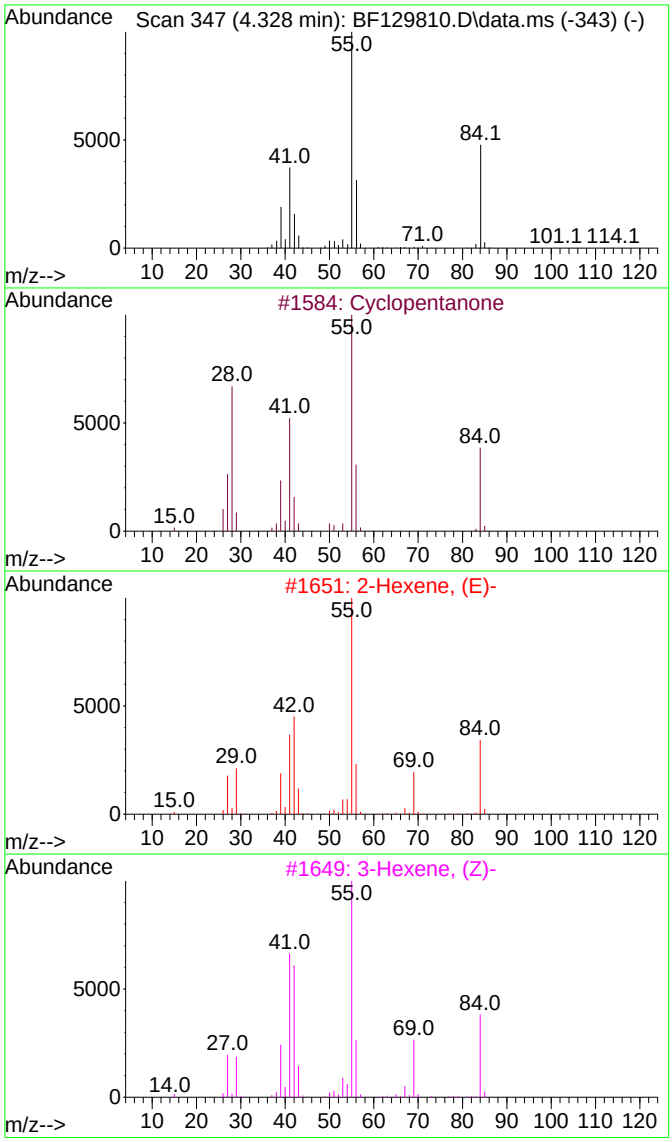
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

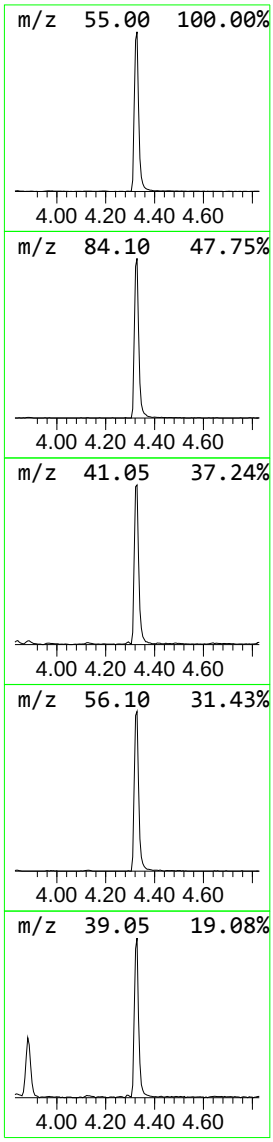
****

Peak Number 2 Cyclopentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.328	19.47 ng	933324	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	91
2	2-Hexene, (E)-	84	C6H12	004050-45-7	72
3	3-Hexene, (Z)-	84	C6H12	007642-09-3	59
4	2-Hexene	84	C6H12	000592-43-8	59
5	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129810.D
Acq On : 16 Aug 2022 14:19
Operator : CG\JU
Sample : N3971-24
Misc :
ALS Vial : 11 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
COP-1R

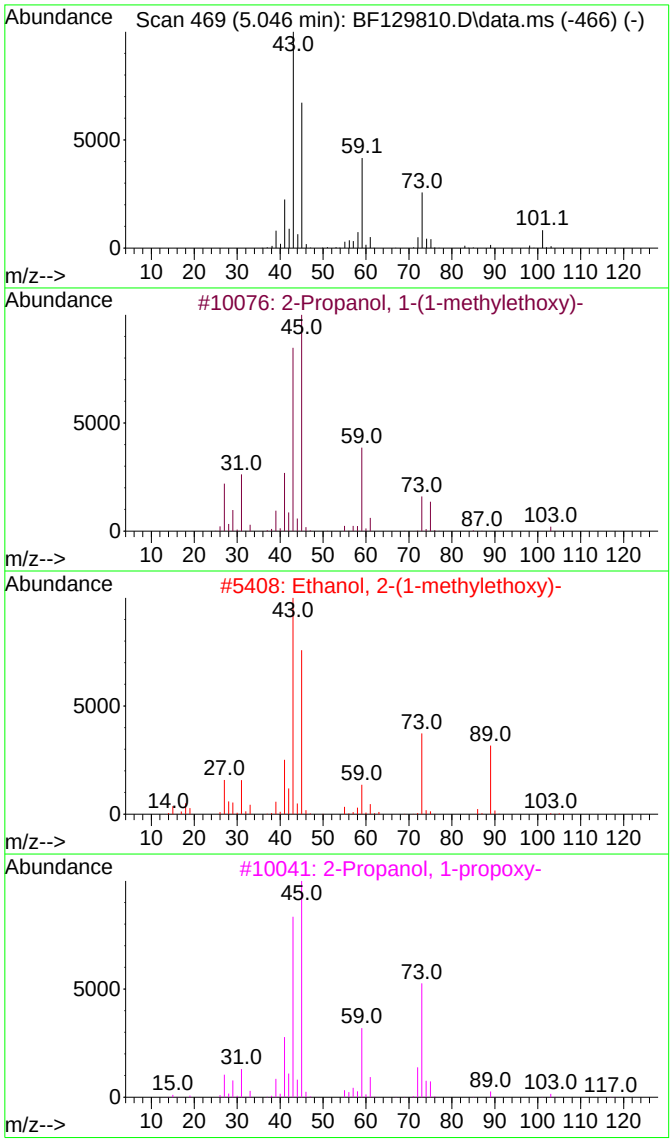
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

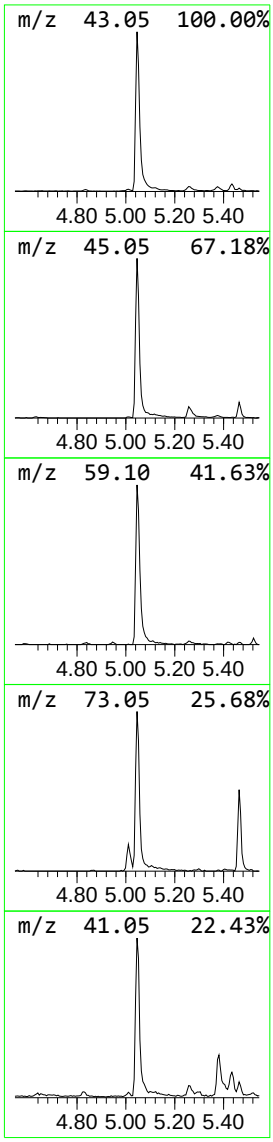
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanol, 1-(1-methyletho... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.046	12.85 ng	615753	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	59
2	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	50
3	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	43
4	Oxirane-2-carboxylic acid, methy...	102	C4H6O3	004538-50-5	42
5	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129810.D
Acq On : 16 Aug 2022 14:19
Operator : CG\JU
Sample : N3971-24
Misc :
ALS Vial : 11 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
COP-1R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

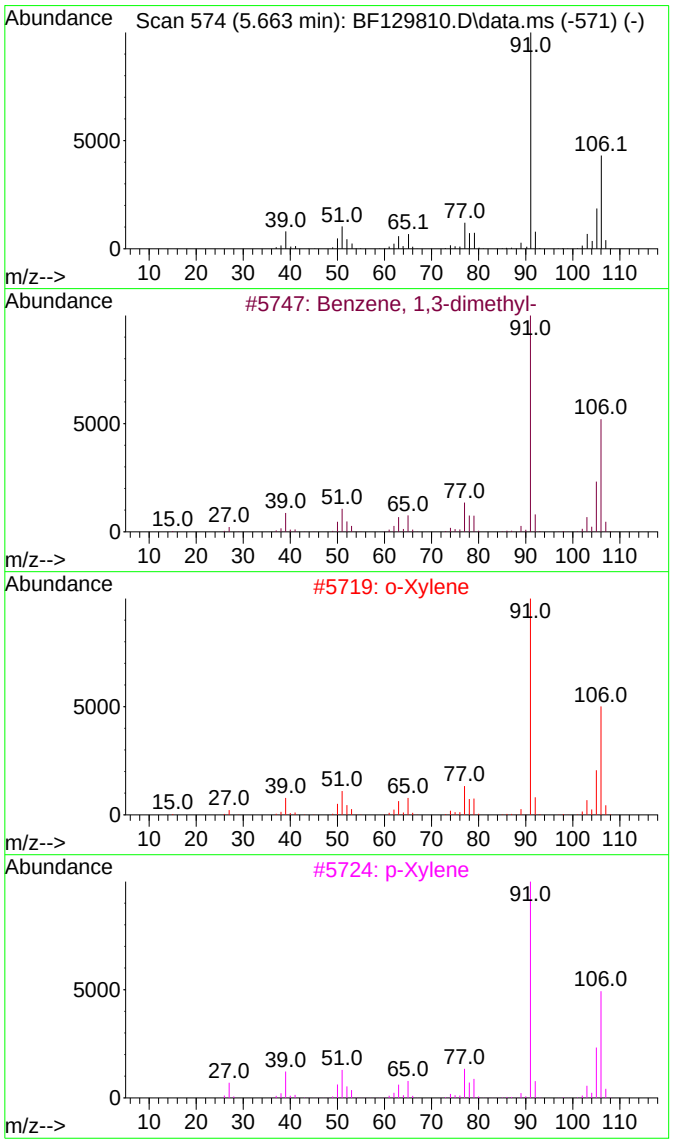
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

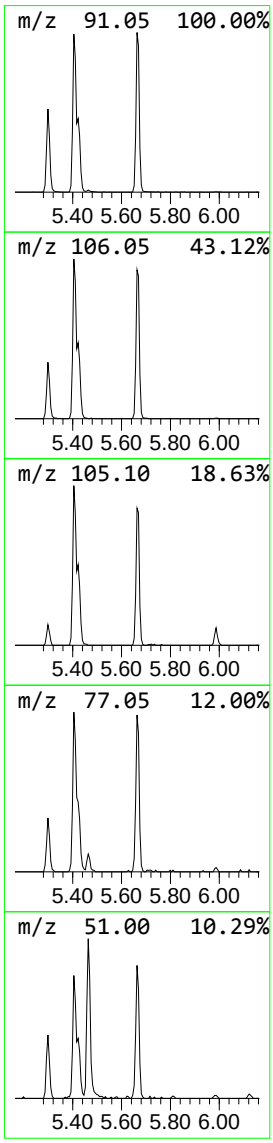
****

Peak Number 5 Benzene, 1,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.663	9.02 ng	432423	1,4-Dichlorobenzene-d4	6.822

Hit# of 4	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	97
2	o-Xylene	106	C8H10	000095-47-6	97
3	p-Xylene	106	C8H10	000106-42-3	97
4	Ethylbenzene	106	C8H10	000100-41-4	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129810.D
Acq On : 16 Aug 2022 14:19
Operator : CG\JU
Sample : N3971-24
Misc :
ALS Vial : 11 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
COP-1R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

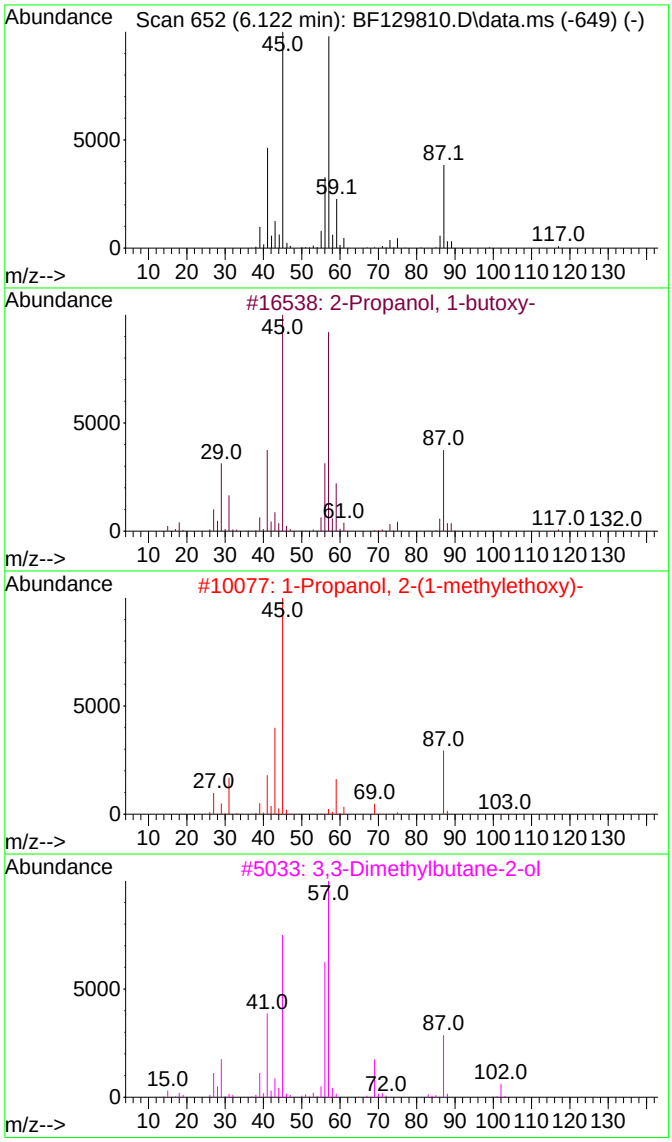
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

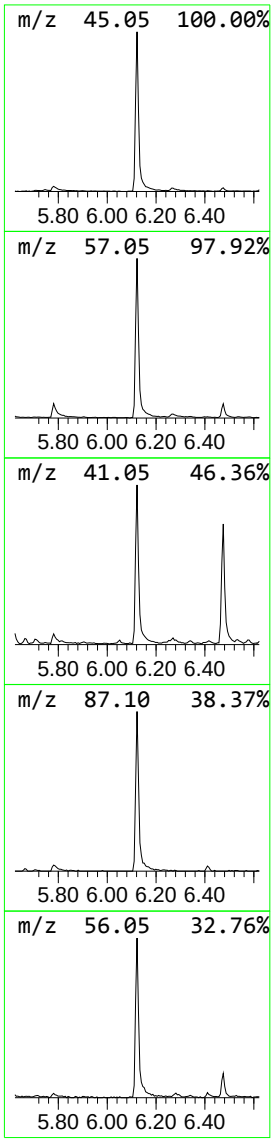
****

Peak Number 6 2-Propanol, 1-butoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.122	10.75 ng	515225	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	90
2	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	59
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
4	Methoxyacetic acid, butyl ester	146	C7H14O3	017640-22-1	47
5	Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129810.D
Acq On : 16 Aug 2022 14:19
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Misc :
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Instrument :
BNA_F
ClientSampleId :
COP-1R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

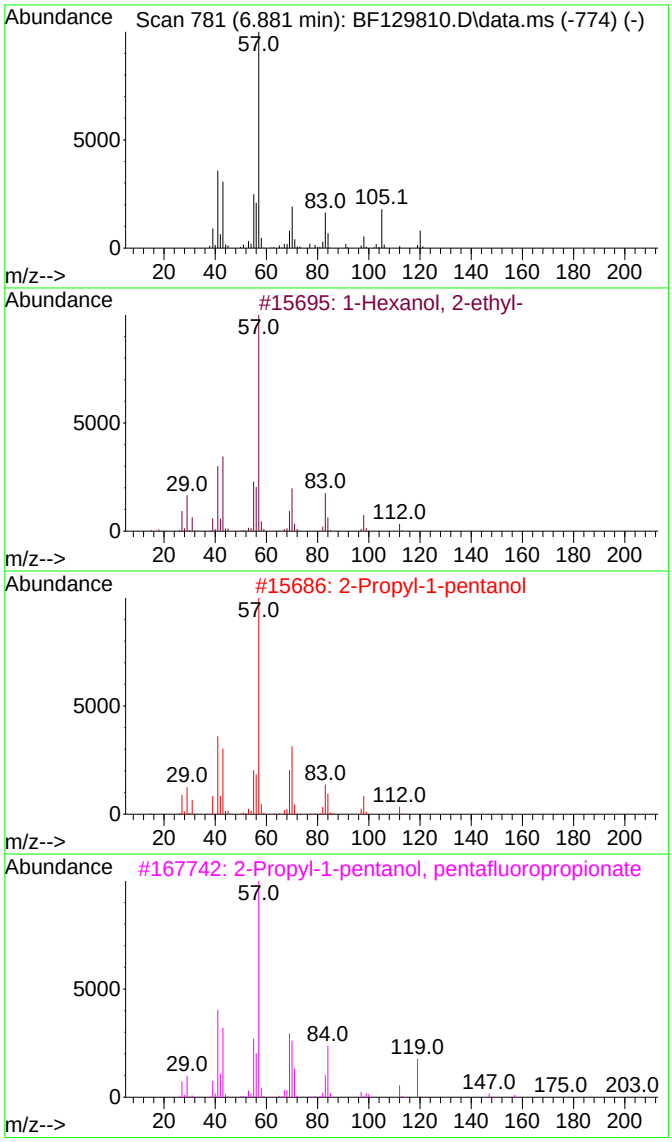
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

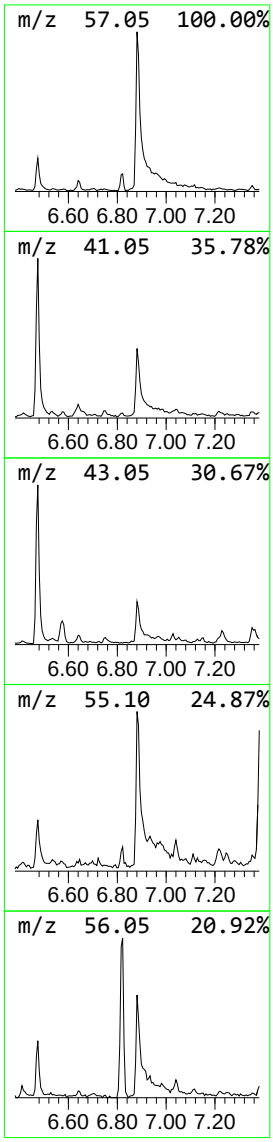
****

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.881	6.04 ng	289535	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
3	2-Propyl-1-pentanol, pentafluoro...	276	C11H17F5O2	1000365-51-2	40
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	40
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	38





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Operator : CG\JU
Sample : N3971-24
Misc :
ALS Vial : 11 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
COP-1R

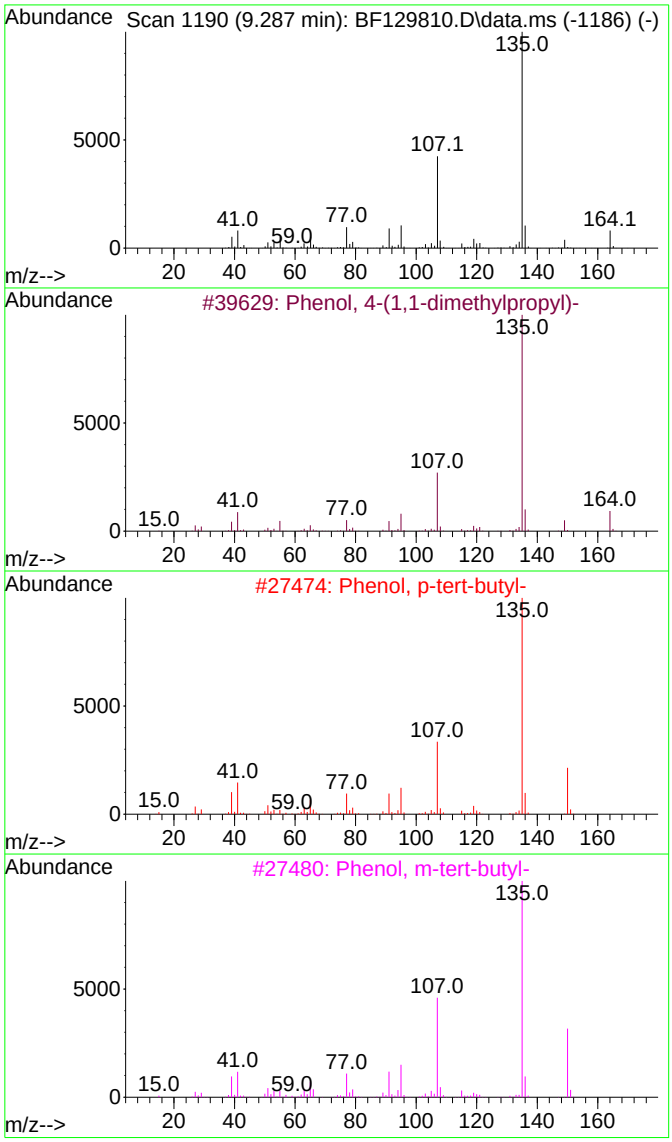
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

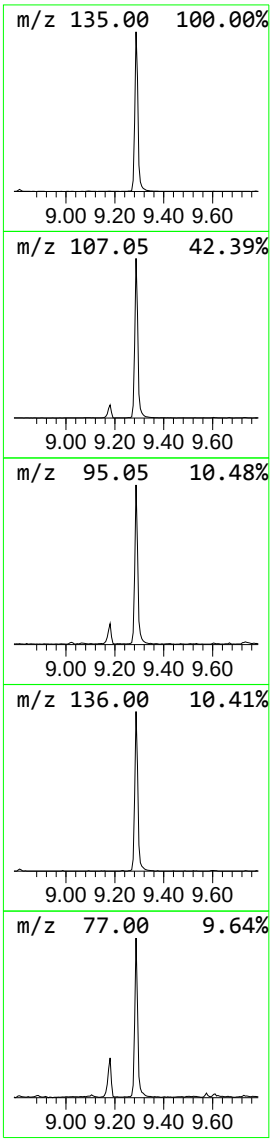
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.287	26.74 ng	2066090	Acenaphthene-d10	9.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	94
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	90
3	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	78
4	4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	64
5	Hexestrol, O-isopropyloxycarbonyl-	356	C22H28O4	1000487-68-4	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129810.D
Acq On : 16 Aug 2022 14:19
Operator : CG\JU
Sample : N3971-24
Misc :
ALS Vial : 11 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
COP-1R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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
Cyclopentanone	4.328	19.5	ng	933324	1	6.822	1917370	20.0
2-Propanol, 1-(...	5.046	12.9	ng	615753	1	6.822	1917370	20.0
Benzene, 1,3-di...	5.663	9.0	ng	432423	1	6.822	1917370	20.0
2-Propanol, 1-b...	6.122	10.8	ng	515225	1	6.822	1917370	20.0
1-Hexanol, 2-et...	6.881	6.0	ng	289535	1	6.822	1917370	20.0
Phenol, 4-(1,1-...	9.287	26.7	ng	2066090	3	9.863	3090100	20.0