LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040822\
Data File : BF127725.D
Acq On : 08 Apr 2022 20:52
Operator : CG\JU
Sample : N2330-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-253

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-BF040622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127725.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.328	3	7	13	rVB	323491	413219	11.89%	1.310%
2	2.440	21	26	35	rVB2	40490	57375	1.65%	0.182%
3	2.681	57	67	73	rVB2	23809	53404	1.54%	0.169%
4	3.716	212	243	245	rBV	571470	3393621	97.63%	10.762%
5	5.204	492	496	502	rVB	208604	241843	6.96%	0.767%
6	5.587	556	561	564	rBV	3029376	3260910	93.82%	10.341%
7	6.587	724	731	734	rBV	3026930	3475865	100.00%	11.023%
8	6.963	789	795	798	rBV	1180200	983682	28.30%	3.119%
9	7.528	885	891	894	rBV	2330791	2238238	64.39%	7.098%
10	8.245	1009	1013	1017	rBV	1330179	1219176	35.08%	3.866%
11	9.328	1191	1197	1200	rBV	3623824	3415560	98.27%	10.832%
12	10.010	1308	1313	1316	rBV	1746267	1426692	41.05%	4.524%
13	10.798	1442	1447	1451	rBV	2803075	2680310	77.11%	8.500%
14	10.974	1474	1477	1479	rBV	67804	52637	1.51%	0.167%
15	11.004	1479	1482	1486	rVV2	55010	66015	1.90%	0.209%
16	11.039	1486	1488	1491	rVV	166127	123687	3.56%	0.392%
17	11.151	1504	1507	1511	rVB3	58237	67357	1.94%	0.214%
18	11.192	1511	1514	1516	rBV	66578	57016	1.64%	0.181%
19	11.304	1530	1533	1540	rBV	45616	61066	1.76%	0.194%
20	11.504	1563	1567	1569	rBV	1623128	1397720	40.21%	4.432%
21	11.521	1569	1570	1574	rVB	59565	43452	1.25%	0.138%
22	12.016	1650	1654	1659	rBV2	175429	201147	5.79%	0.638%
23	12.480	1729	1733	1740	rBV	70930	107789	3.10%	0.342%
24	12.716	1770	1773	1778	rBV	138962	123600	3.56%	0.392%
25	12.945	1807	1812	1815	rBV	101659	126752	3.65%	0.402%
26	13.092	1830	1837	1840	rBV	3353261	2899804	83.43%	9.196%
27	13.510	1905	1908	1916	rBV	73802	132246	3.80%	0.419%
28	13.621	1924	1927	1930	rBV	70868	65766	1.89%	0.209%
29	13.980	1984	1988	1998	rVB	380846	408865	11.76%	1.297%
30	14.121	2009	2012	2014	rBV	286019	255902	7.36%	0.812%
31	14.151	2014	2017	2020	rVV	1049909	935080	26.90%	2.965%
32	14.174	2020	2021	2028	rVB	63381	43352	1.25%	0.137%
33	14.245	2030	2033	2038	rVB2	47696	60499	1.74%	0.192%
34	14.621	2093	2097	2102	rBV3	61073	77998	2.24%	0.247%
35	15.215	2195	2198	2202	rBV	51108	82345	2.37%	0.261%
36	15.298	2209	2212	2215	rBV2	34278	40150	1.16%	0.127%

LSC Area Percent Report

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Sample : N2330-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-253

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-BF040622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.327	2215	2217	2223	rVB4	27895	37146	1.07%	0.118%
38	15.539	2250	2253	2261	rVB	37568	55831	1.61%	0.177%
39	15.604	2261	2264	2268	rBV	40708	50727	1.46%	0.161%
40	15.680	2271	2277	2281	rBV	651289	873564	25.13%	2.770%
41	16.180	2358	2362	2366	rVB3	28224	40304	1.16%	0.128%
42	16.233	2367	2371	2376	rBV6	32518	51702	1.49%	0.164%
43	16.721	2449	2454	2459	rBV4	26105	49084	1.41%	0.156%
44	17.227	2536	2540	2549	rVB4	22092	49275	1.42%	0.156%
45	17.703	2616	2621	2629	rVB2	15723	35737	1.03%	0.113%

Sum of corrected areas: 31533510

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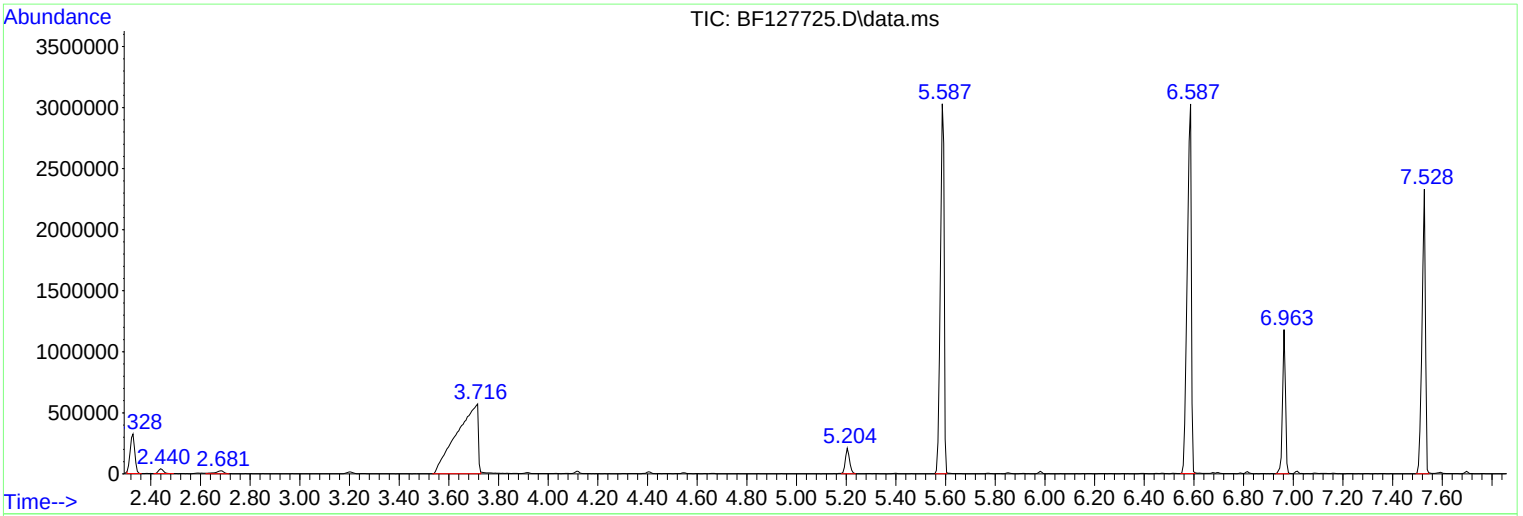
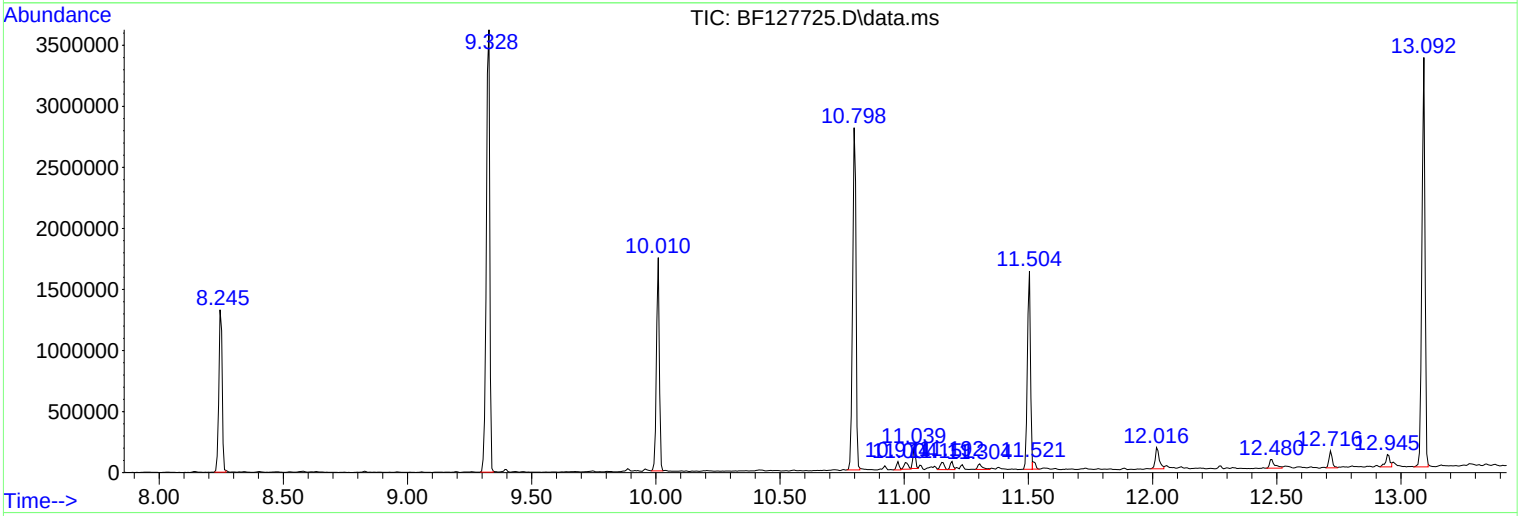
Misc :
ALS Vial : 21 Sample Multiplier: 1

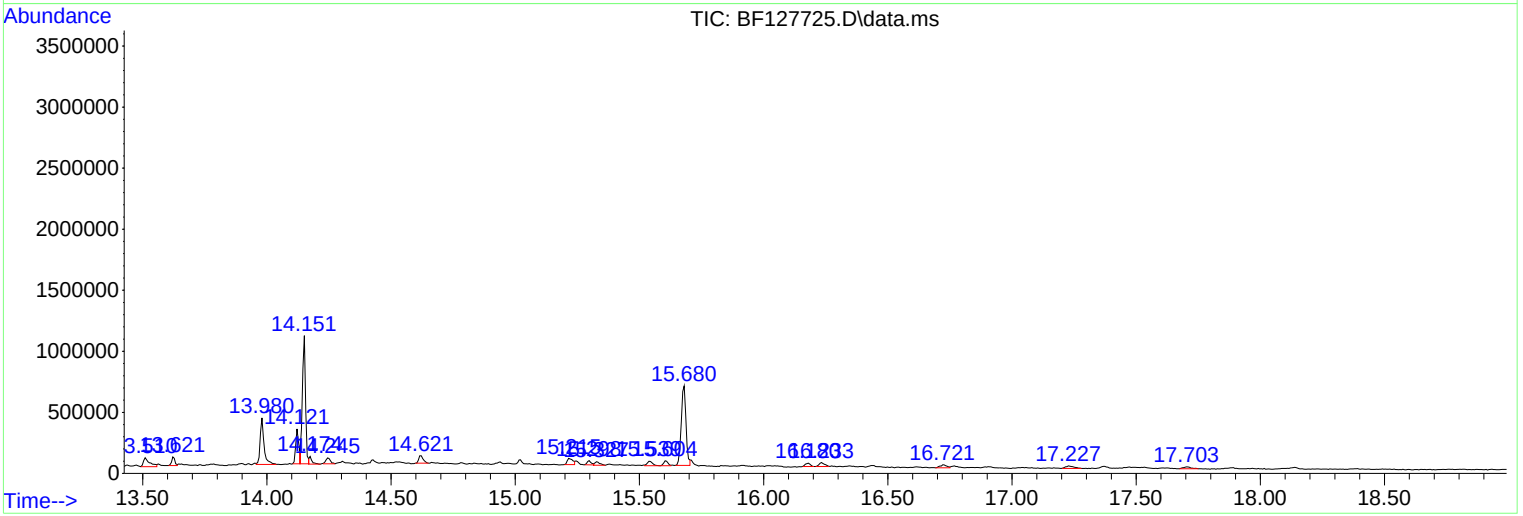
Instrument :
BNA_F
ClientSampleId :
RBR-253

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.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\BF040822\
Data File : BF127725.D
Acq On : 08 Apr 2022 20:52
Operator : CG\JU
Sample : N2330-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-253

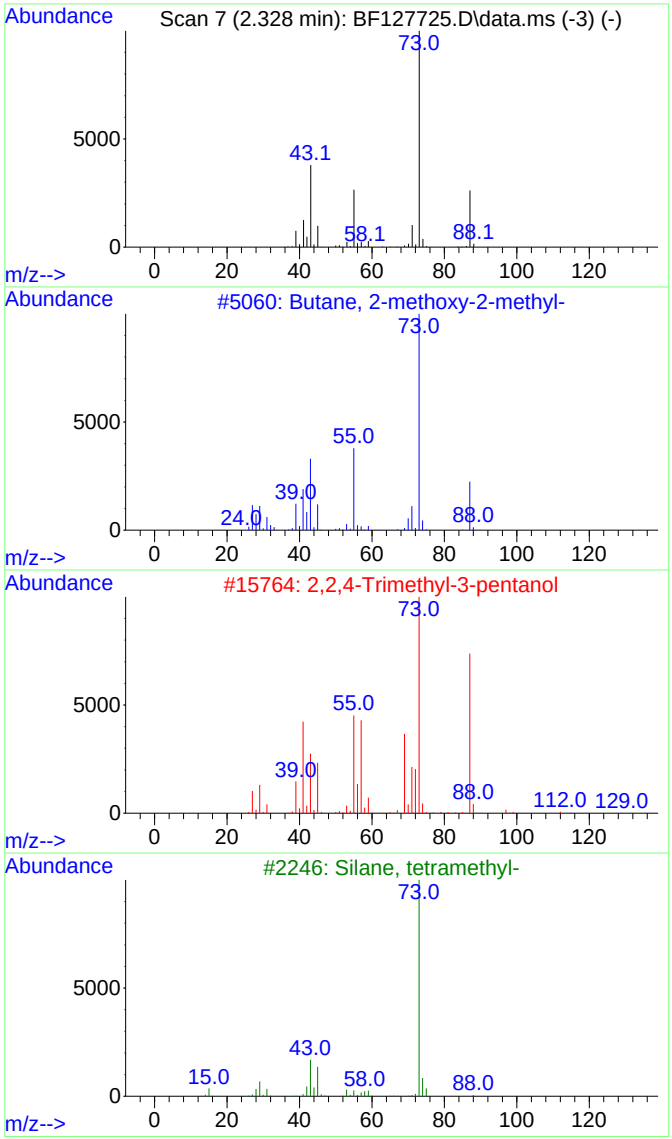
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

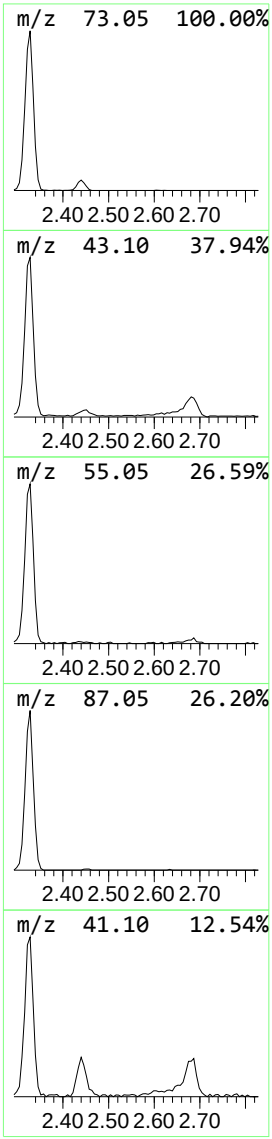
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.328	8.40 ng	413219	1,4-Dichlorobenzene-d4	6.963

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	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Data File : BF127725.D
Acq On : 08 Apr 2022 20:52
Operator : CG\JU
Sample : N2330-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-253

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

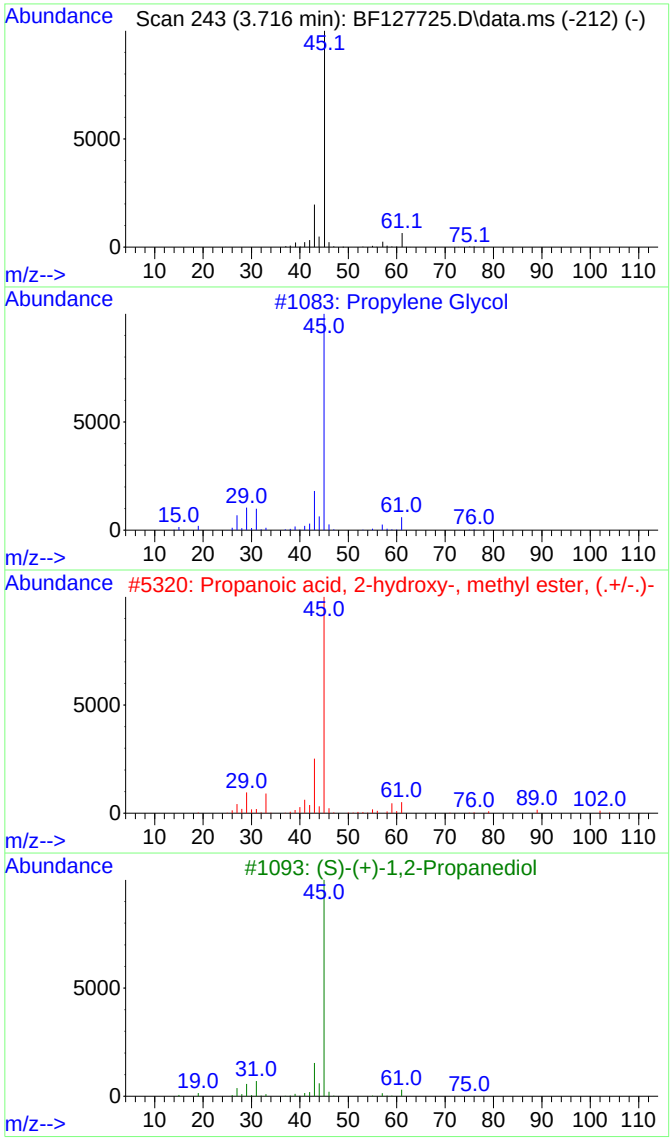
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

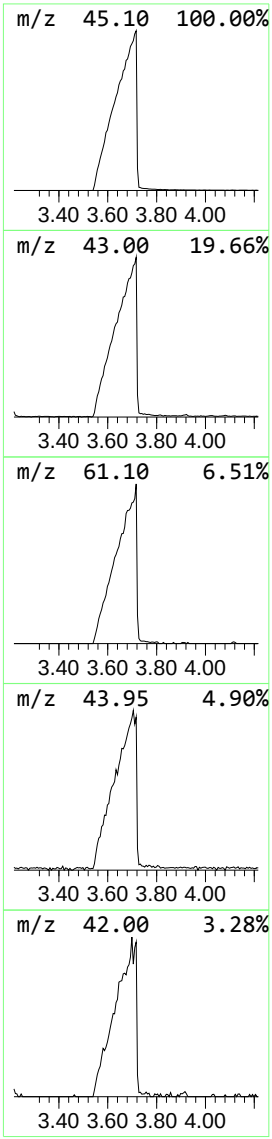
****

Peak Number 2 Propylene Glycol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.716	69.00 ng	3393620	1,4-Dichlorobenzene-d4	6.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	86
2	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	9





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Operator : CG\JU
Sample : N2330-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-253

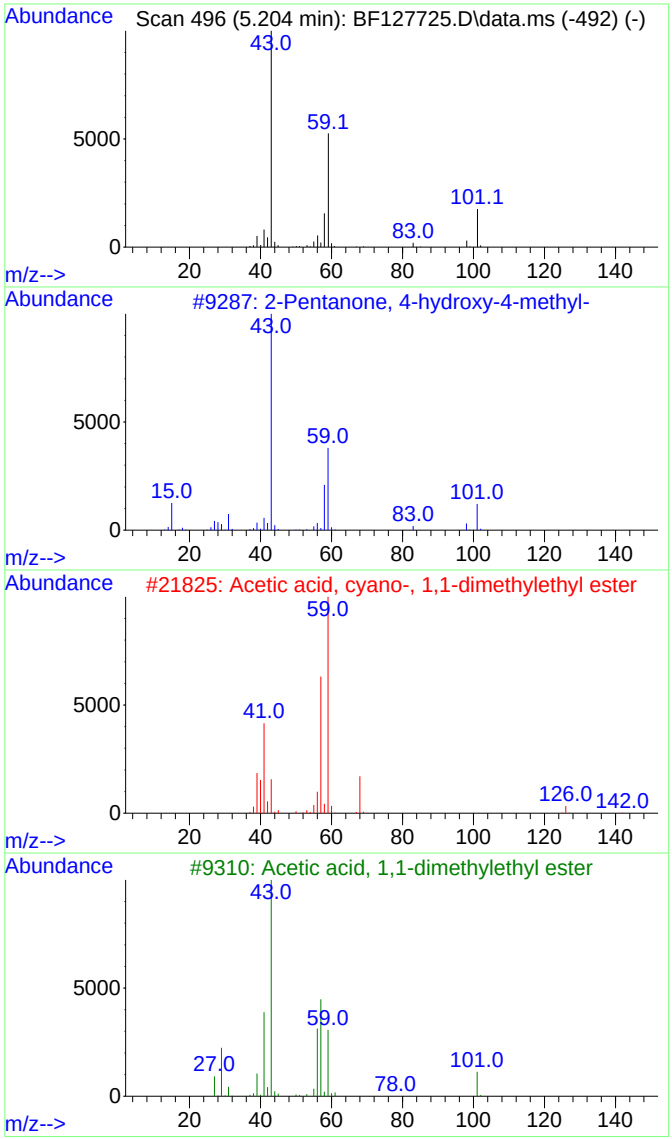
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

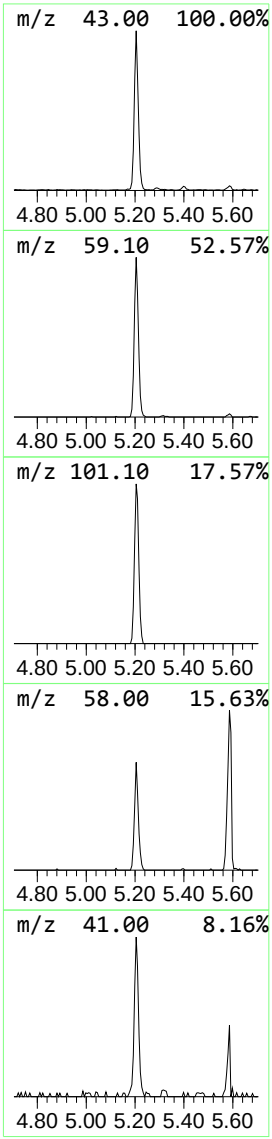
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.204	4.92 ng	241843	1,4-Dichlorobenzene-d4	6.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040822\
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Operator : CG\JU
Sample : N2330-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-253

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

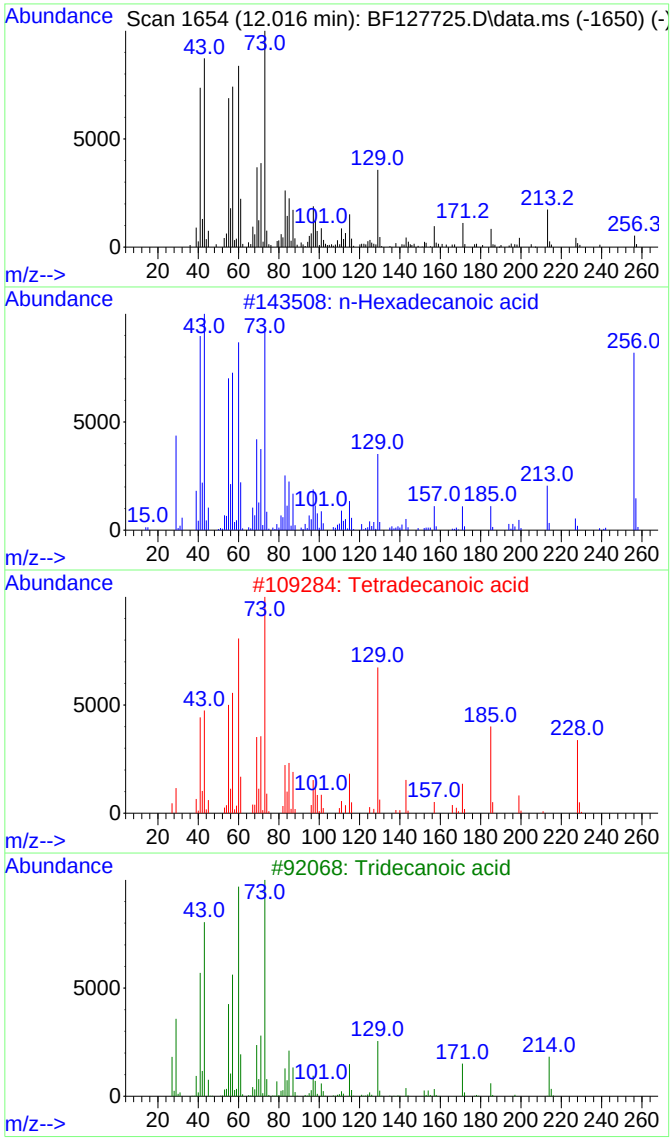
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

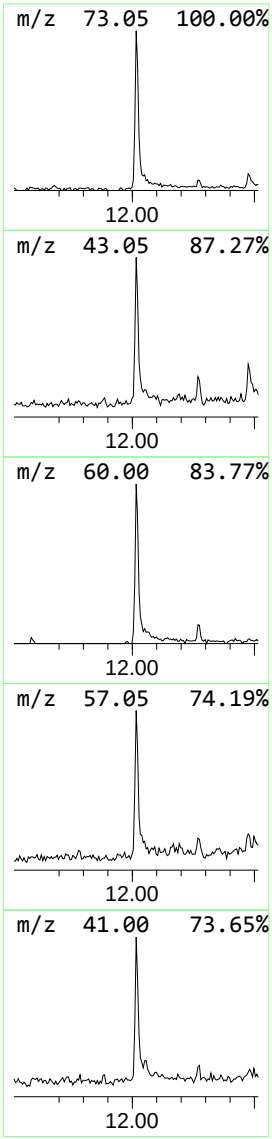
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.016	2.88 ng	201147	Phenanthrene-d10	11.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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Instrument :
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ClientSampleId :
RBR-253

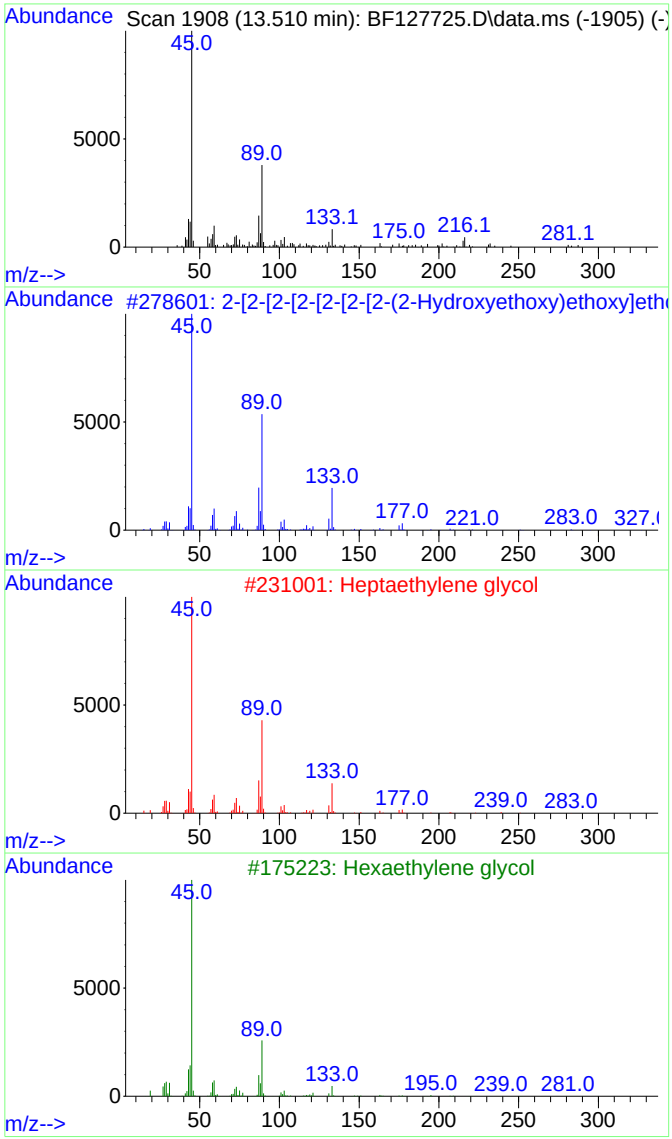
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

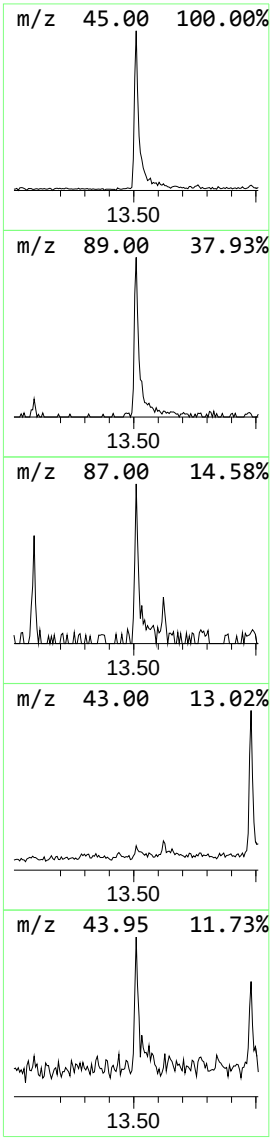
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-[2-[2-[2-[2-[2-[2-(2-Hydr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.510	2.83 ng	132246	Chrysene-d12	14.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	87
2	Heptaethylene glycol	326	C14H30O8	005617-32-3	87
3	Hexaethylene glycol	282	C12H26O7	002615-15-8	86
4	Pentaethylene glycol	238	C10H22O6	004792-15-8	86
5	2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	003386-18-3	86





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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-253

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

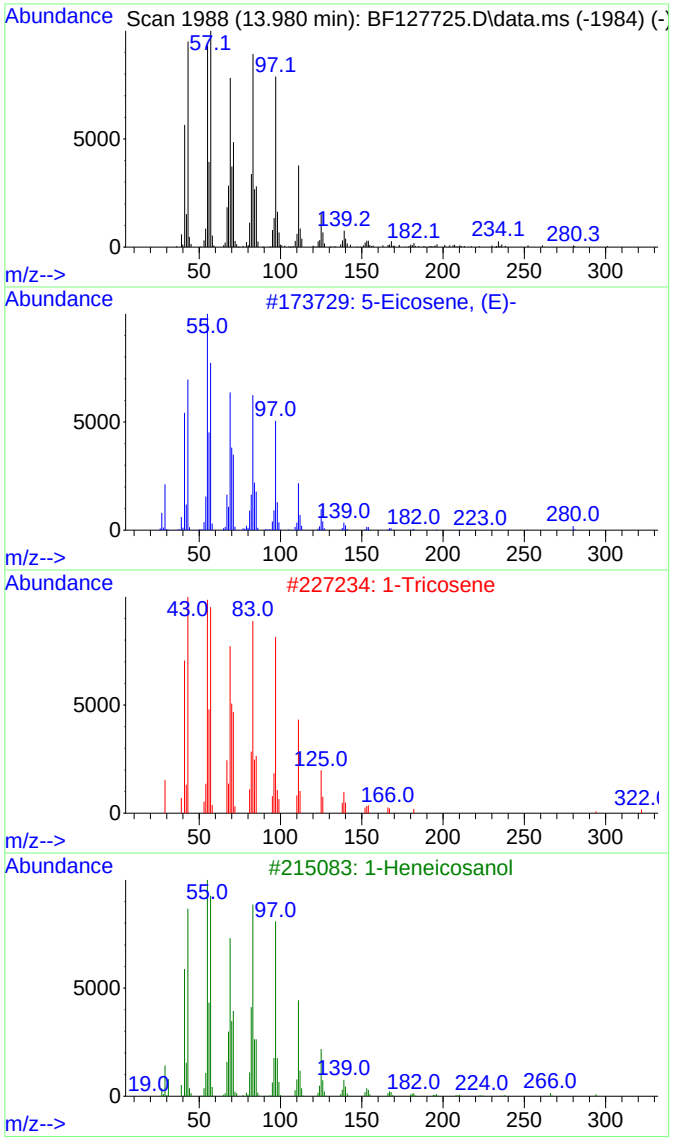
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

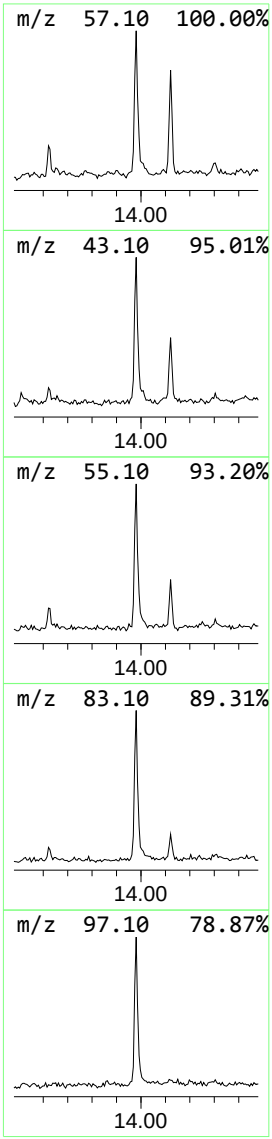
****

Peak Number 7 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.980	8.75 ng	408865	Chrysene-d12	14.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2	1-Tricosene	322	C23H46	018835-32-0	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	1-Hexacosene	364	C26H52	018835-33-1	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040822\
Data File : BF127725.D
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Sample : N2330-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-253

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.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...	2.328	8.4	ng	413219	1	6.963	983682	20.0
Propylene Glycol	3.716	69.0	ng	3393620	1	6.963	983682	20.0
2-Pentanone, 4-...	5.204	4.9	ng	241843	1	6.963	983682	20.0
n-Hexadecanoic ...	12.016	2.9	ng	201147	4	11.504	1397720	20.0
2-[2-[2-[2-[2-[...	13.510	2.8	ng	132246	5	14.151	935080	20.0
5-Eicosene, (E)-	13.980	8.8	ng	408865	5	14.151	935080	20.0